Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Design, synthesis and structure-activity relationships of mangostin analogs as cytotoxic agents

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List of supplementary material

Abbreviation for the manuscript

DCM	Dichloromethane
DMF	Dimethylformamide
BrBn	Benzyl bromide
DMAP	4-Dimethylaminopyridine
Ac_2O	Acetic anhydride
$(CH_3)_2SO_4$	Dimethyl sulfate
$BrCH_2CHCH_2$	3-Bromopropene
$BrCH_2CHC(CH_3)_2$	1-Bromo-3-methyl-2-butene
OsO_4	Osmium tetroxide
NMO	4-Methylmorpholine-N-oxide
DDQ	2,3-Dicyano-5,6-dichlorobenzoquinone

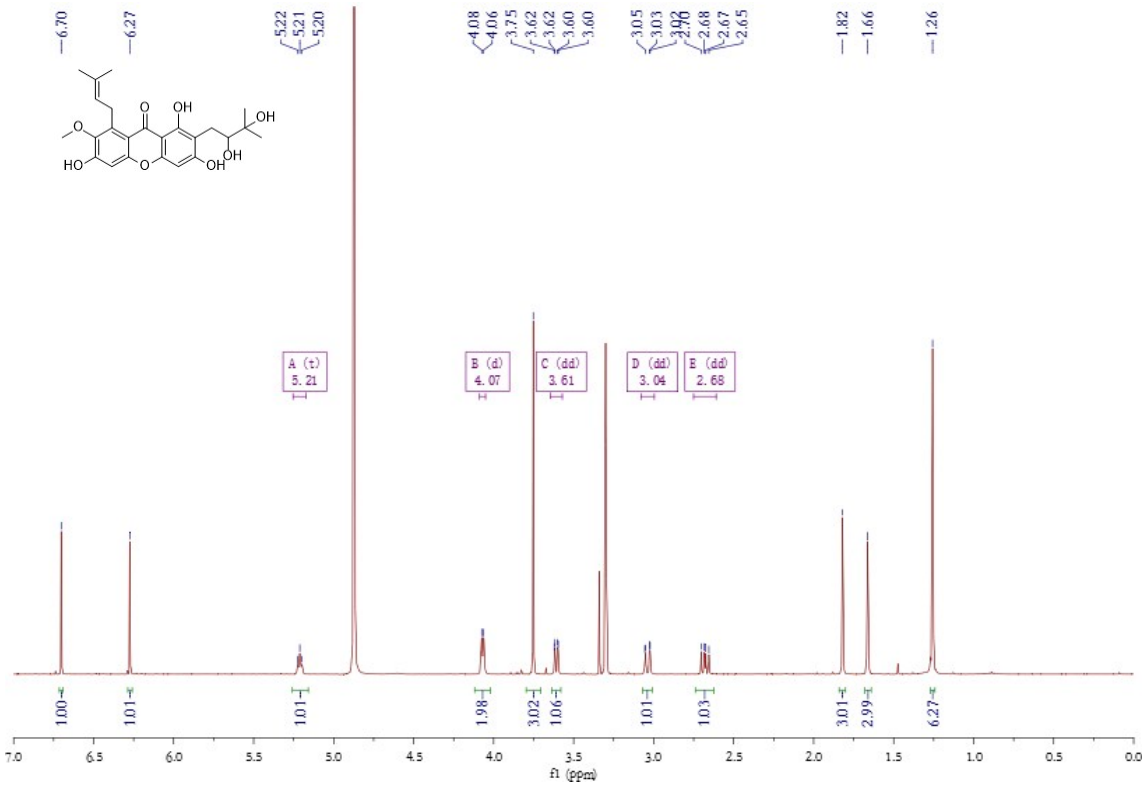


Figure 1S. ^{1}H NMR spectrum (CD_3OD, 500 MHz) of compound **2a**

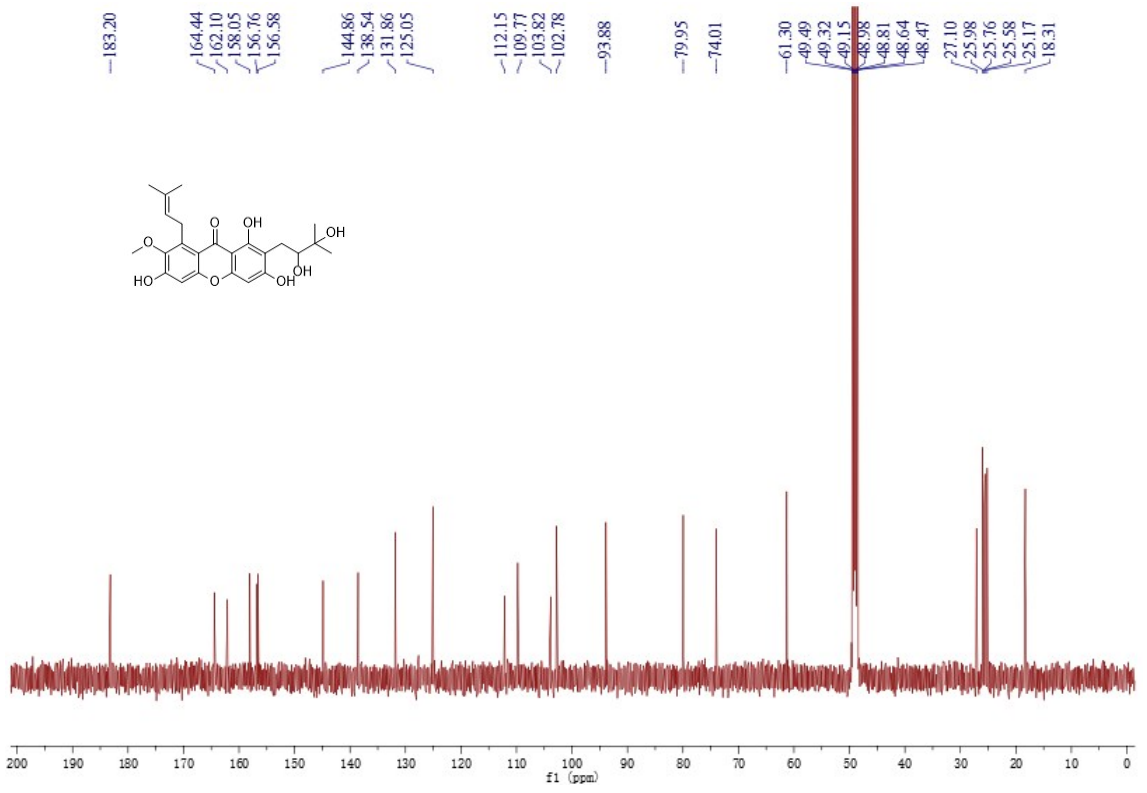


Figure 2S. ^{13}C NMR spectrum (CD_3OD, 125 MHz) of compound **2a**

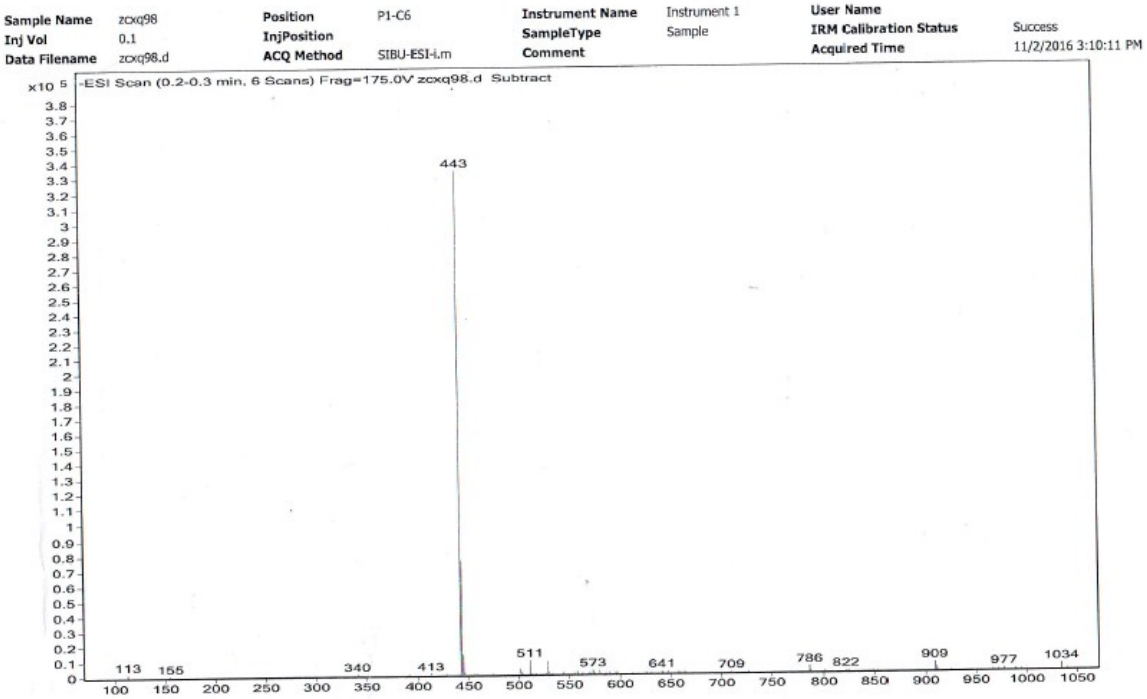


Figure 3S. Negative ESI-MS spectrum of compound **2a**

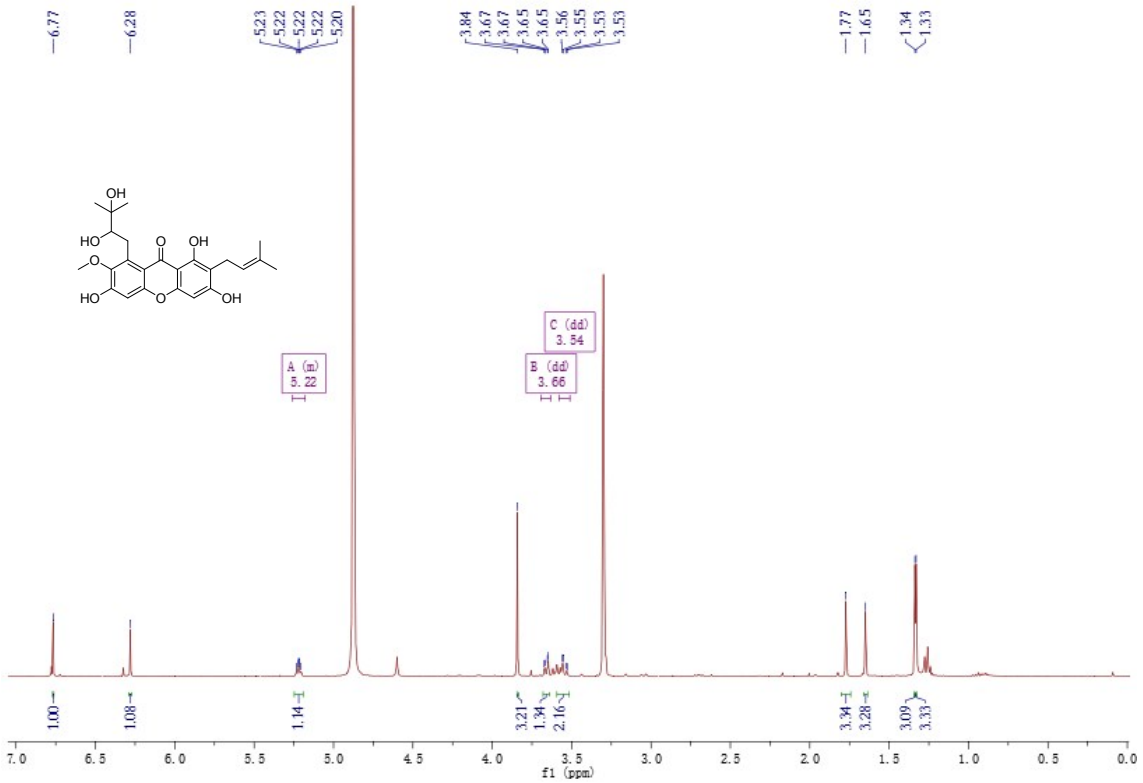


Figure 4S. ^{1}H NMR spectrum (CD_3OD, 500 MHz) of compound **2b**

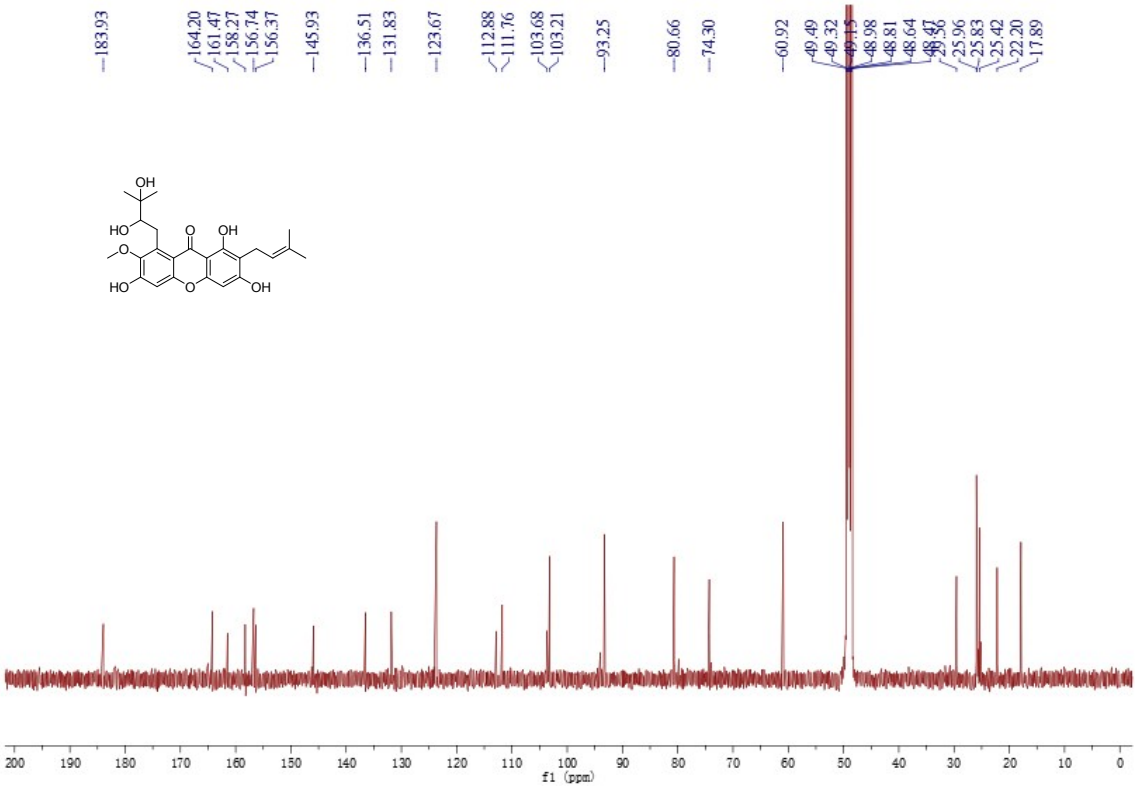


Figure 5S. ^{13}C NMR spectrum (CD_3OD, 125 MHz) of compound **2b**

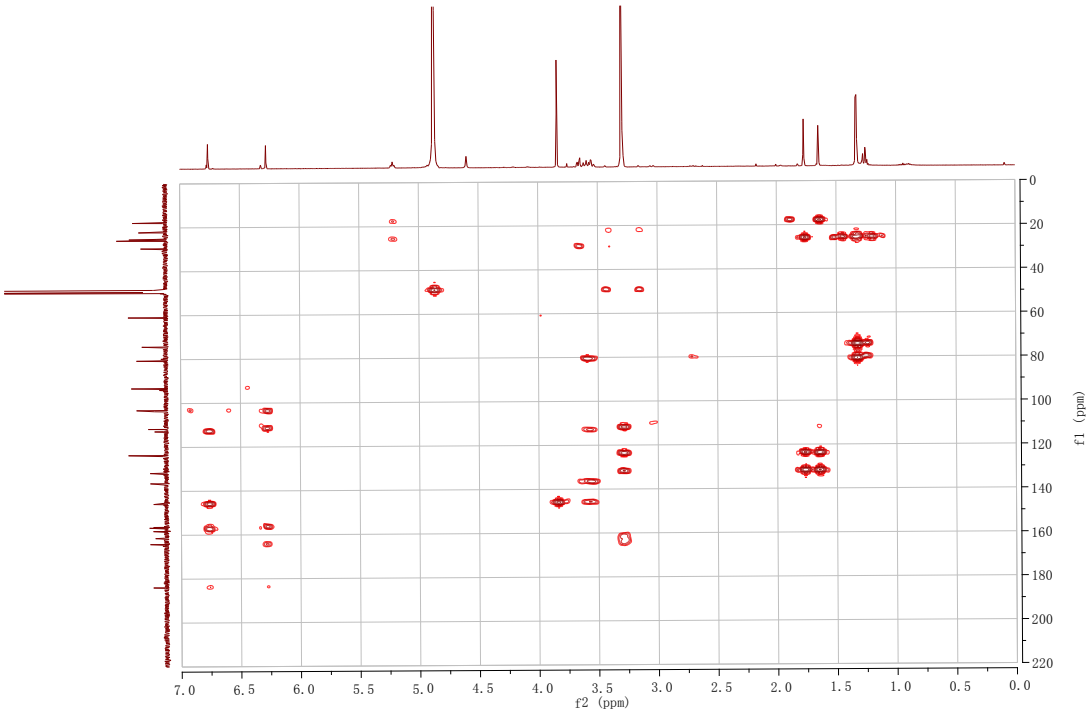


Figure 6S. HMBC spectrum (CD_3OD, 125 MHz) of compound **2b**

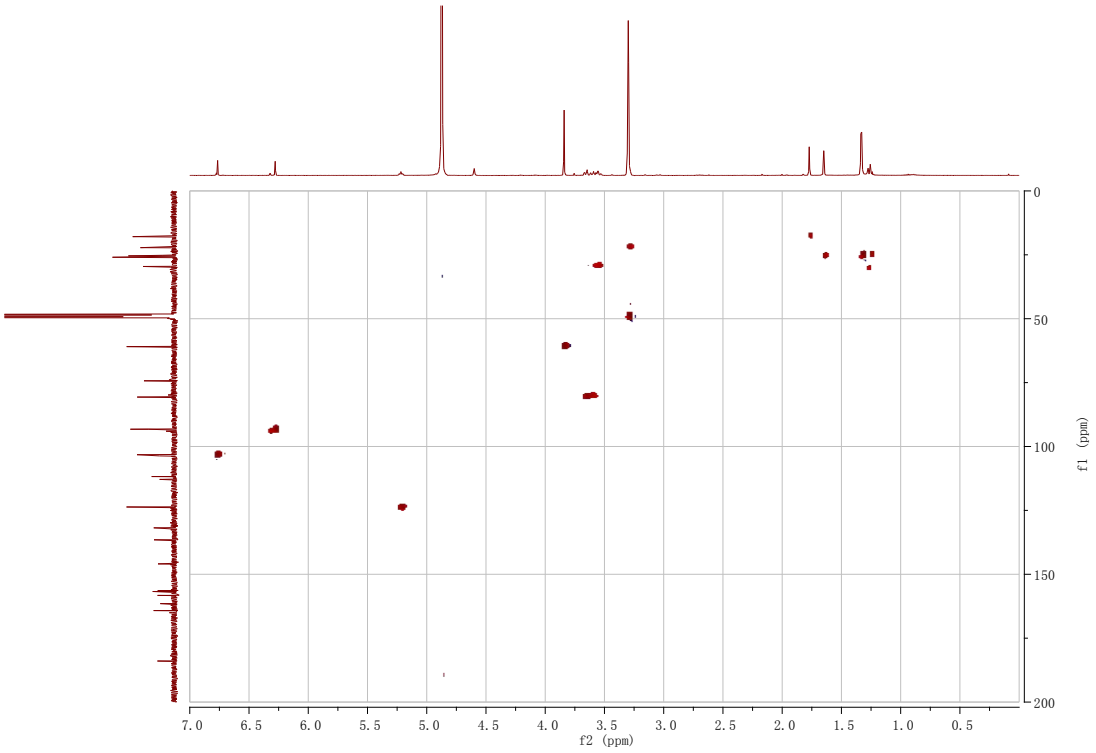


Figure 7S. HSQC spectrum (CD_3OD, 125 MHz) of compound **2b**

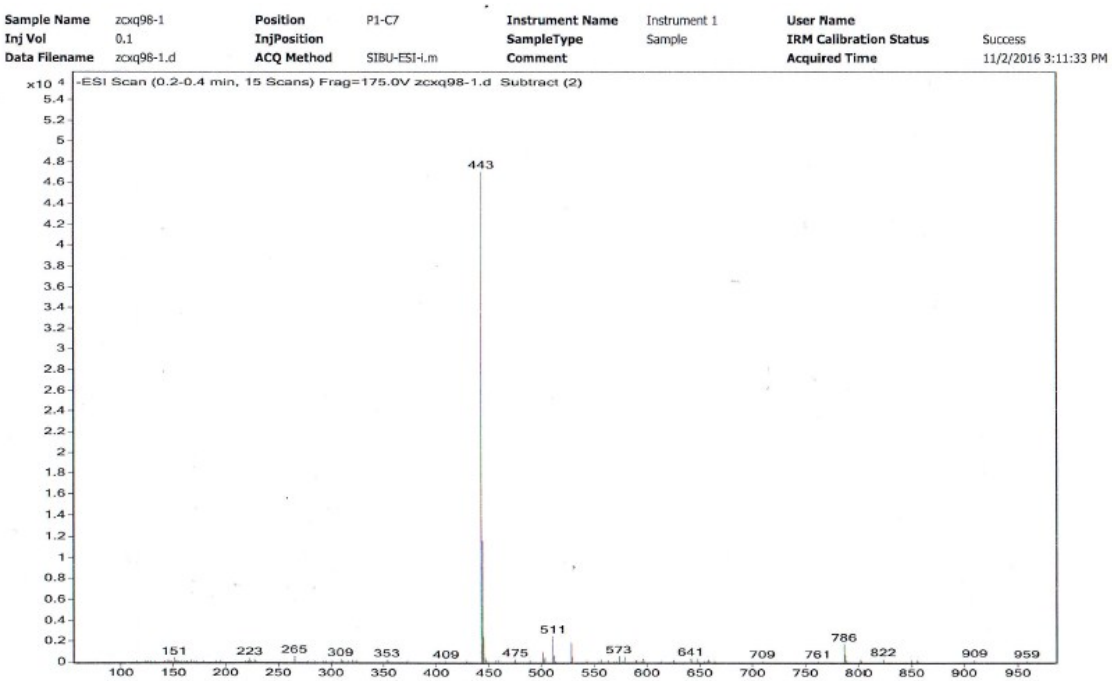


Figure 8S. Negative ESI-MS spectrum of compound **2b**

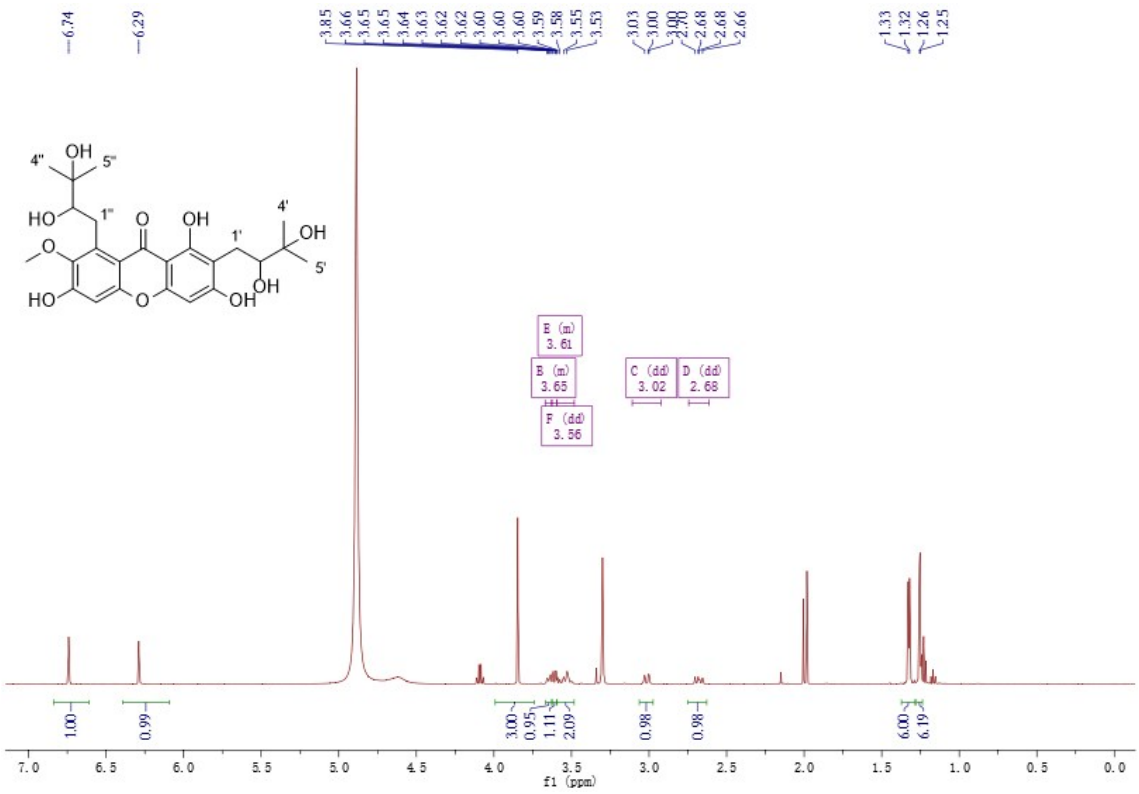


Figure 9S. ^{1}H NMR spectrum (CD_3OD, 500 MHz) of compound **2c**

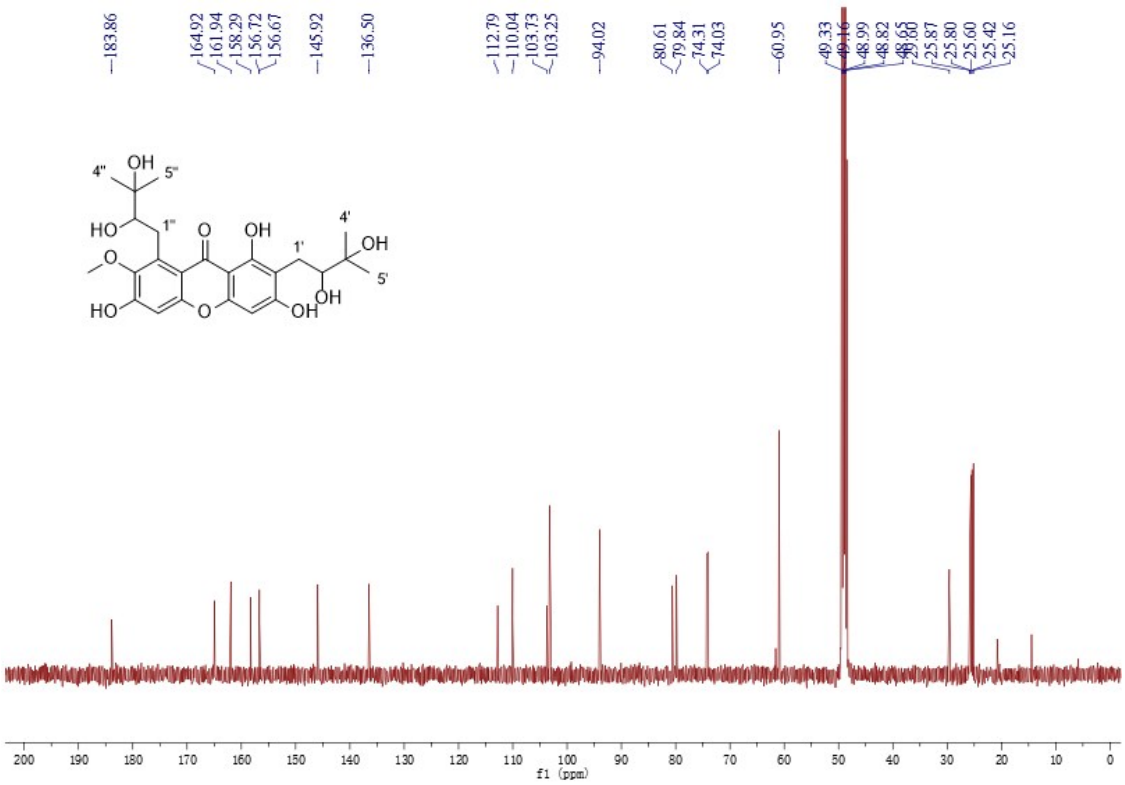


Figure 10S. ^{13}C NMR spectrum (CD_3OD, 125 MHz) of compound **2c**

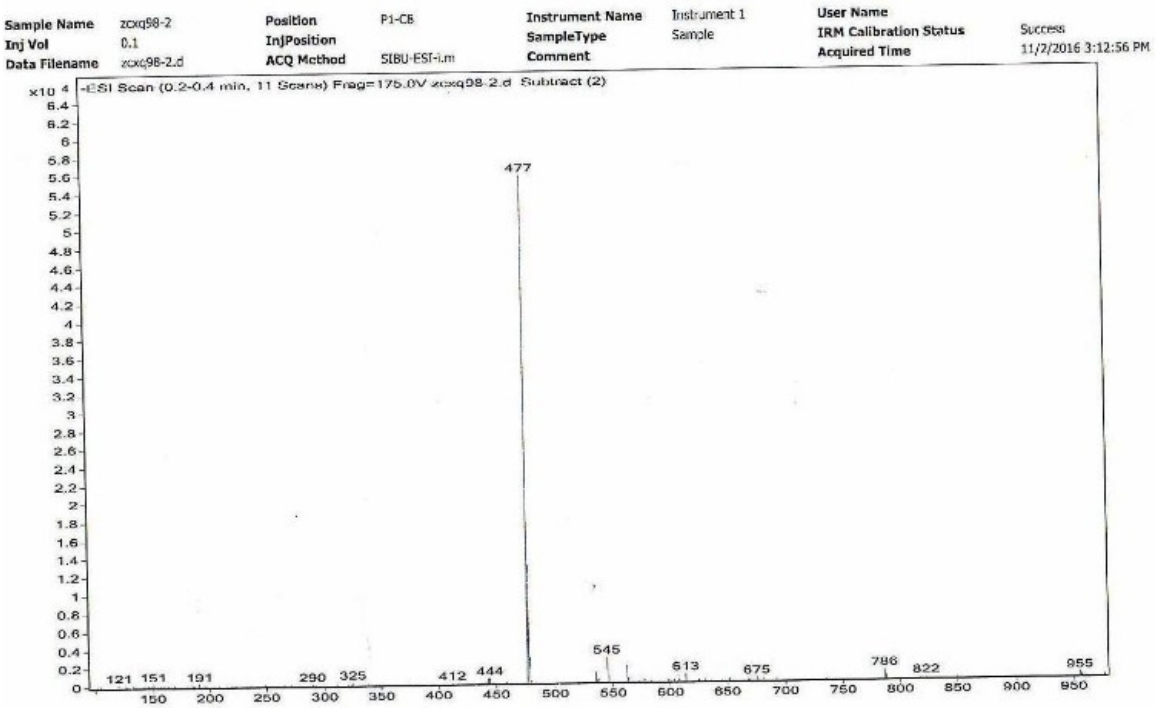


Figure 11S. Negative ESI-MS spectrum of compound **2c**

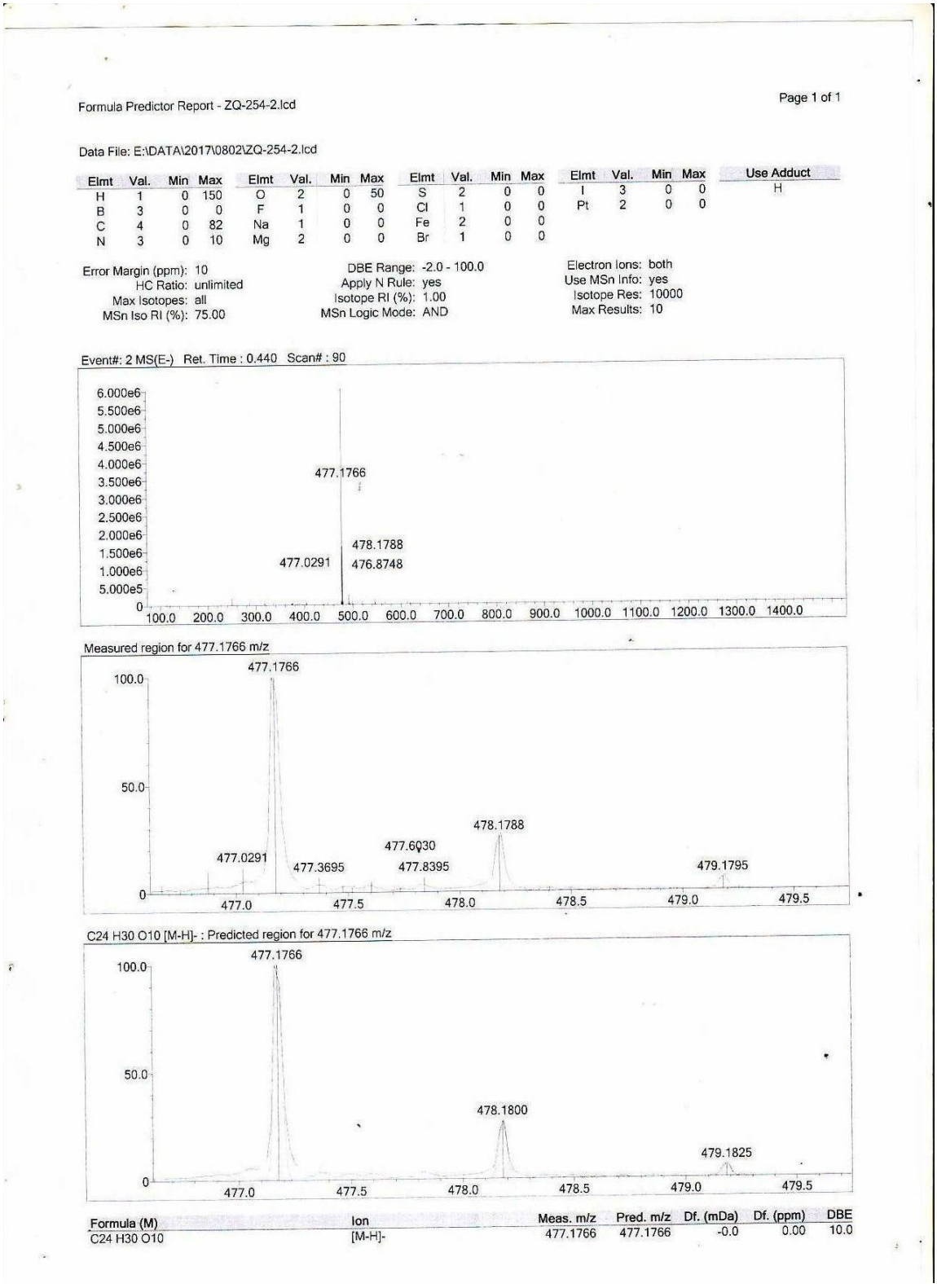


Figure 12S. Negative HR-ESIMS spectrum of compound **2c**

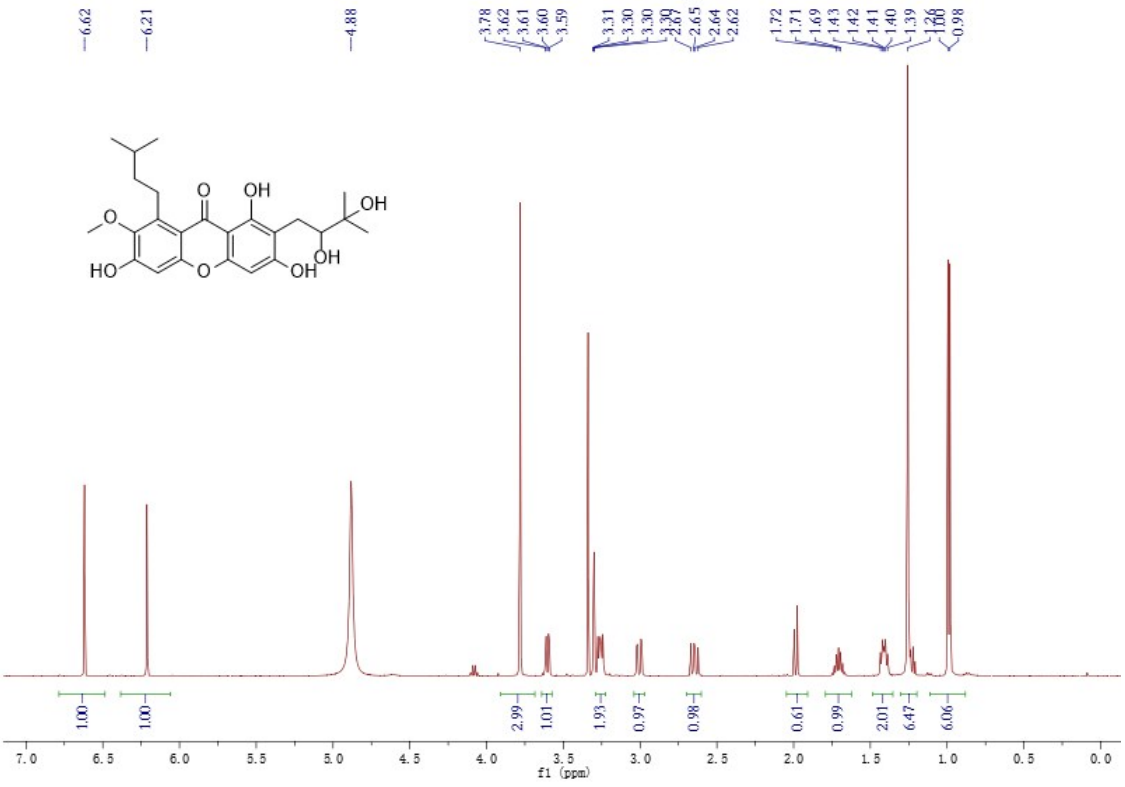


Figure 13S. ^{1}H NMR spectrum (CD_3OD, 500 MHz) of compound **2d**

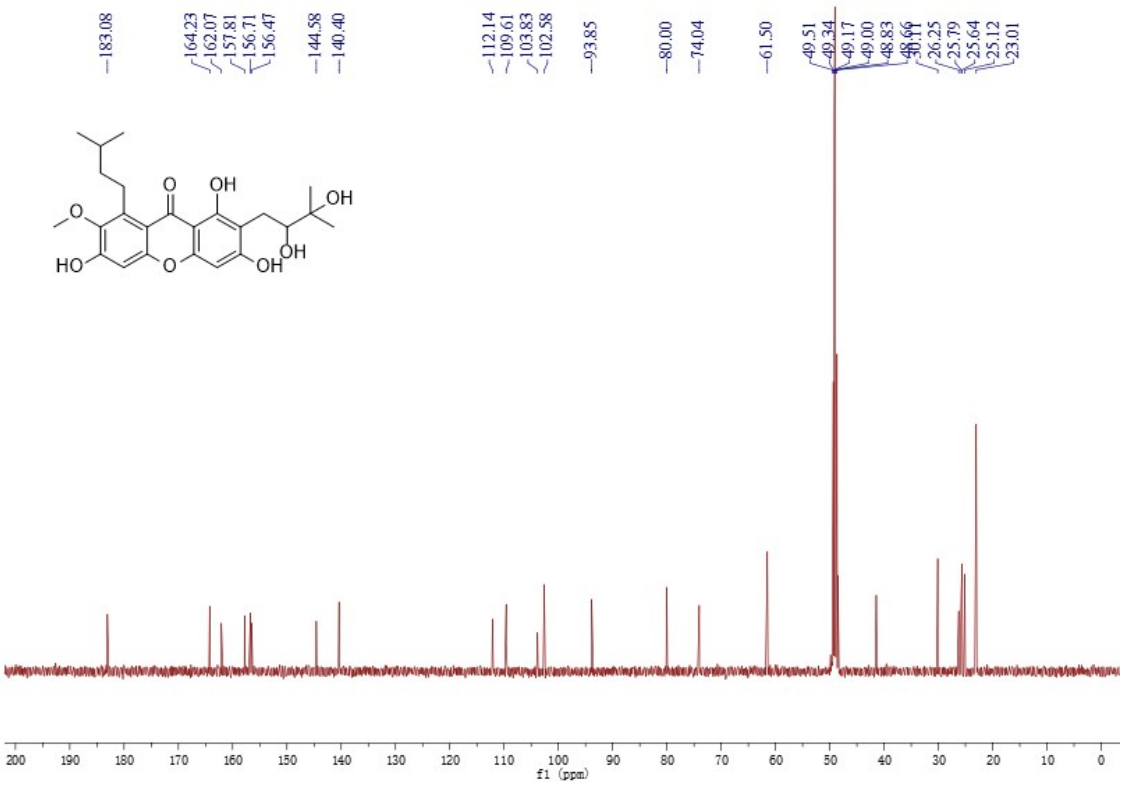


Figure 14S. ^{13}C NMR spectrum (CD_3OD, 125 MHz) of compound **2d**

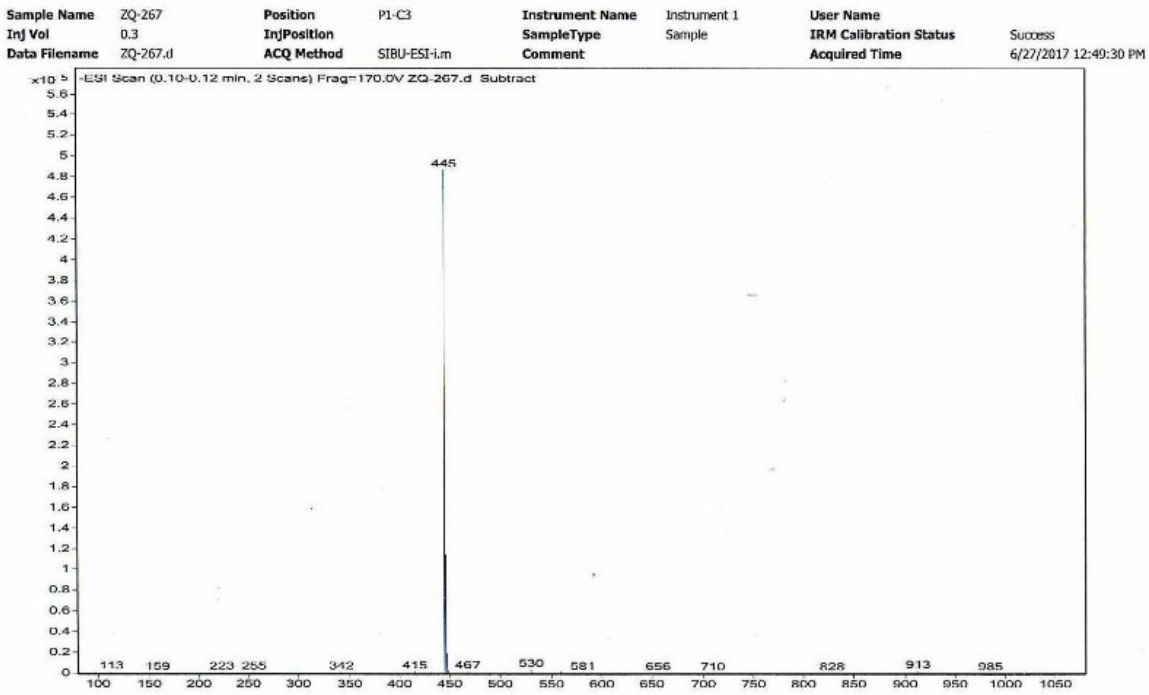


Figure 15S. Negative ESI-MS spectrum of compound **2d**

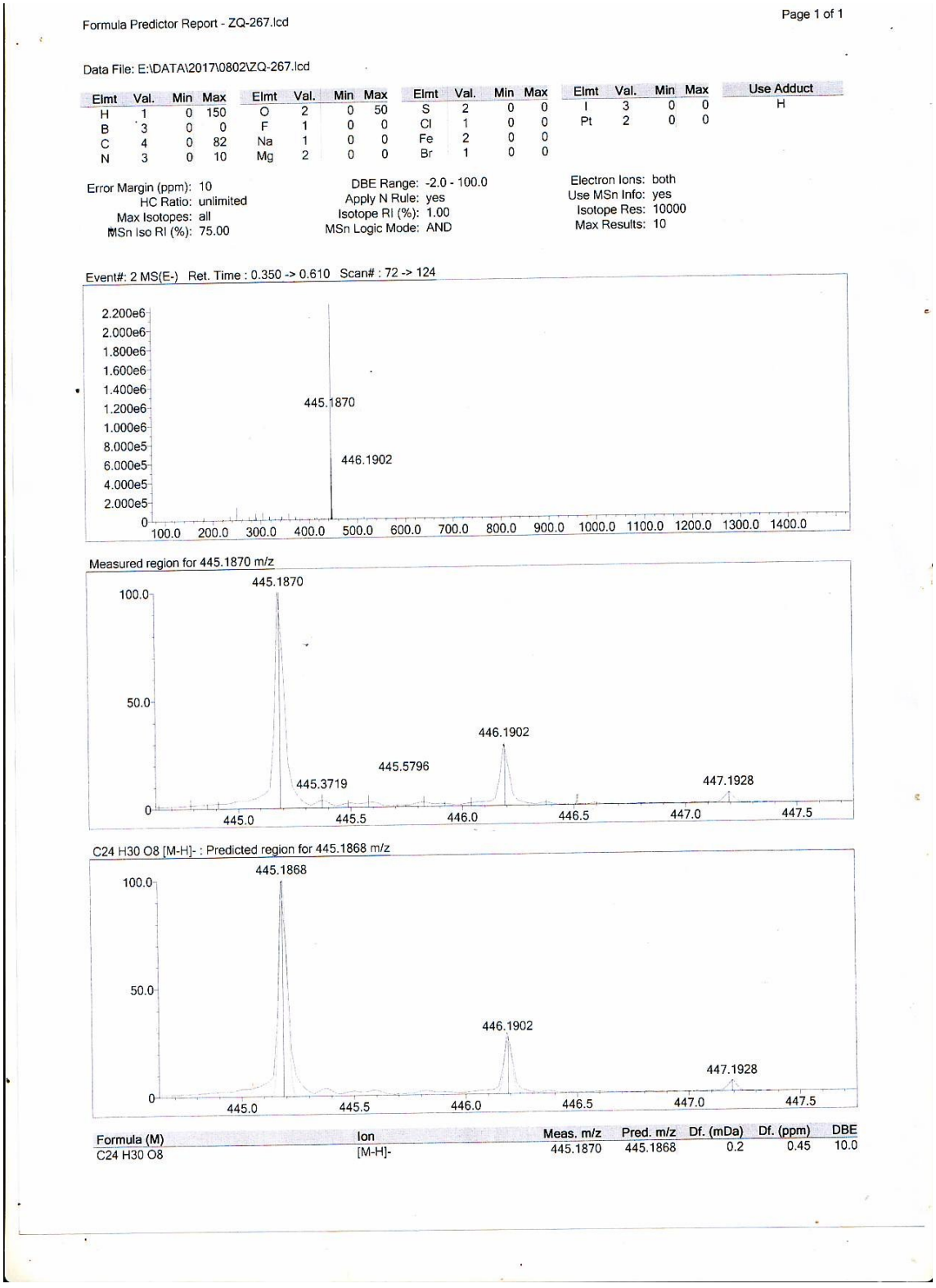


Figure 16S. Negative HR-ESIMS spectrum of compound **2d**

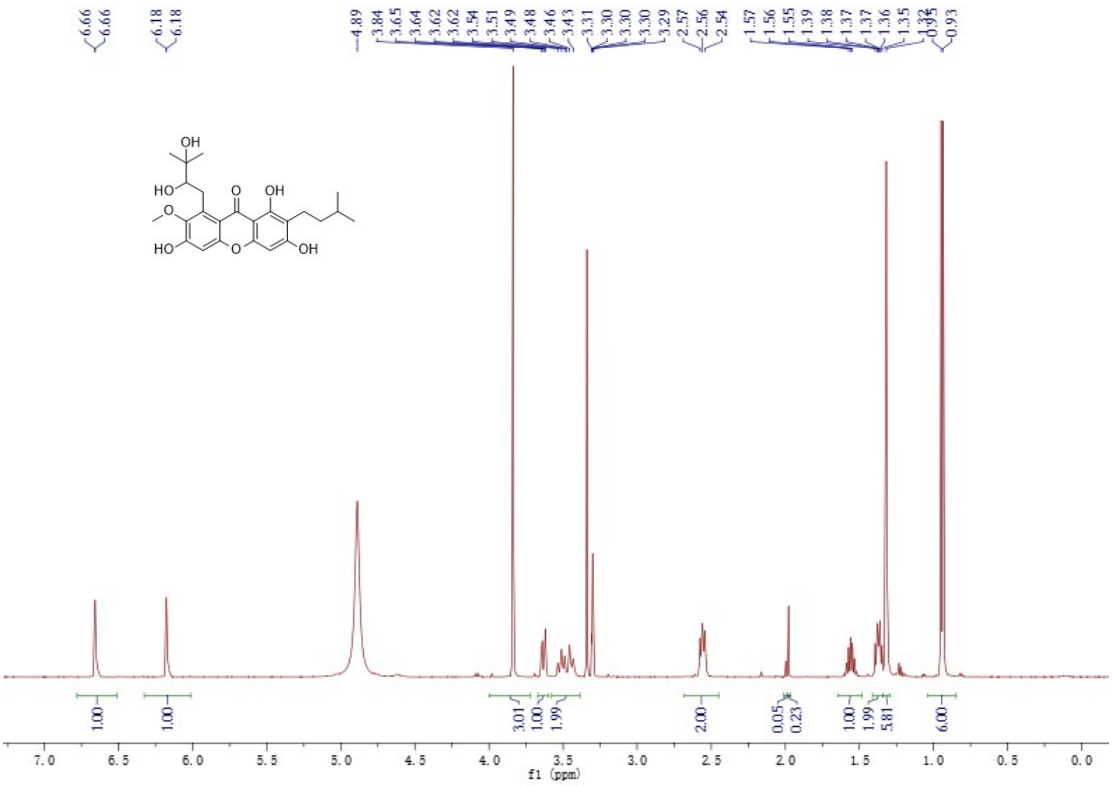


Figure 17S. ^{1}H NMR spectrum (CD_3OD, 500 MHz) of compound **2e**

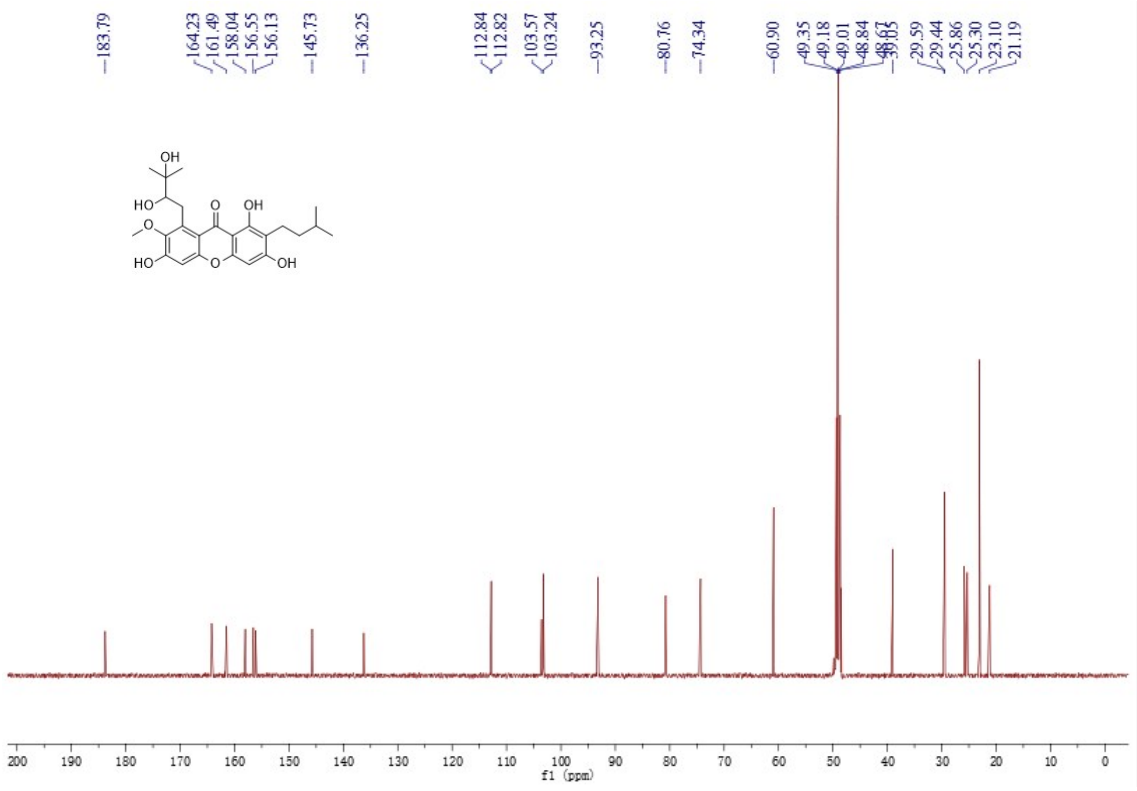


Figure 18S. ^{13}C NMR spectrum (CD_3OD, 125 MHz) of compound **2e**

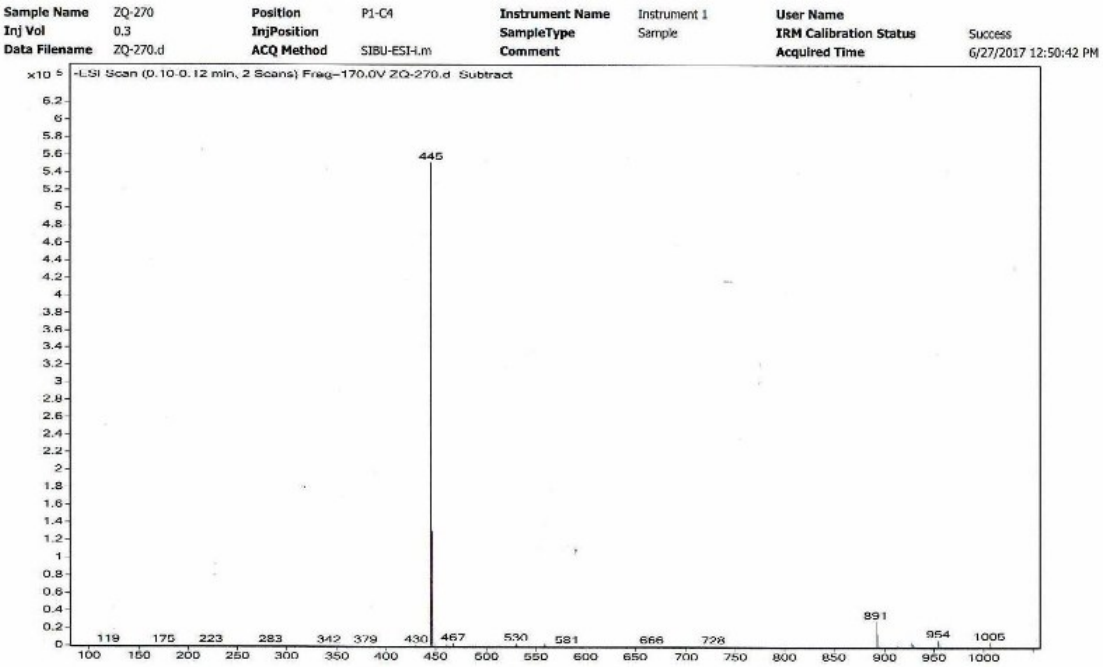


Figure 19S. Negative ESI-MS spectrum of compound **2e**

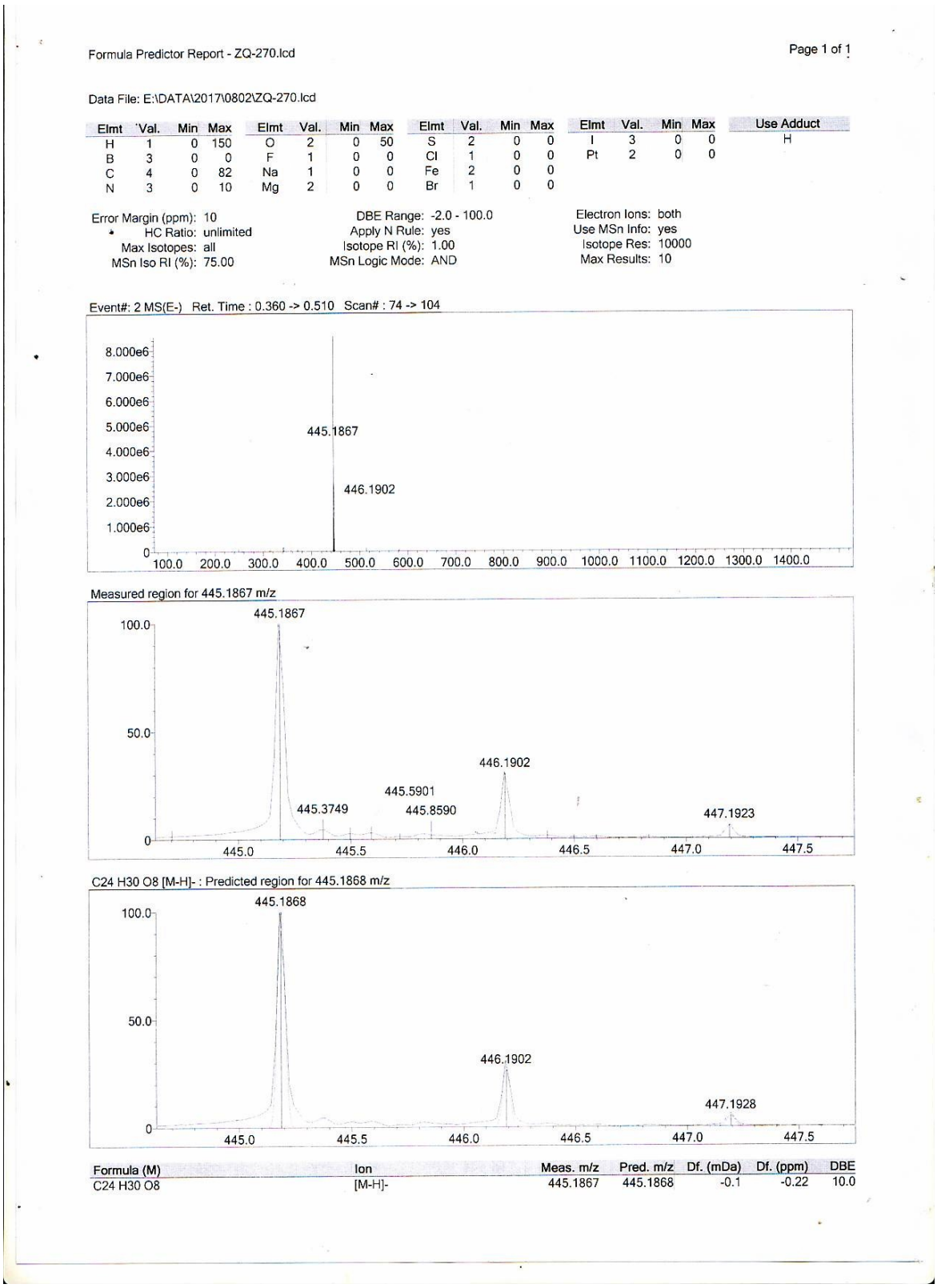


Figure 20S. Negative HR-ESIMS spectrum of compound **2e**

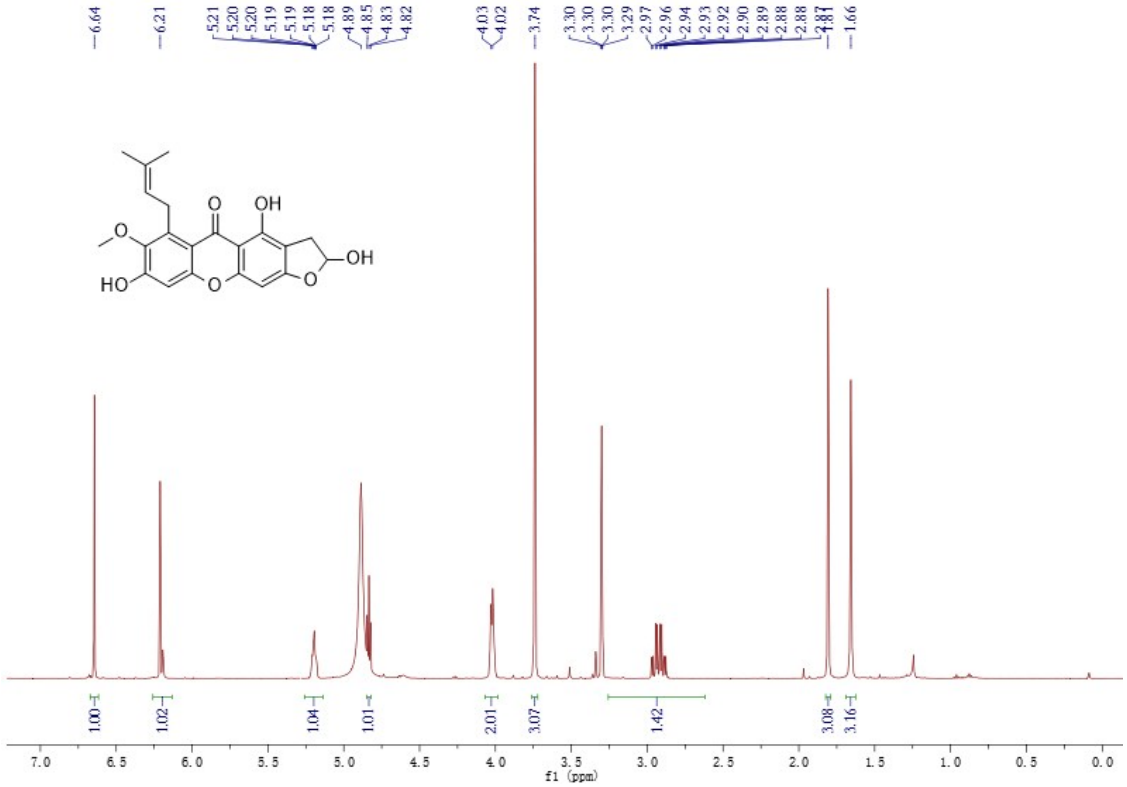


Figure 21S. ^{1}H NMR spectrum (CD_3OD, 500 MHz) of compound **2f**

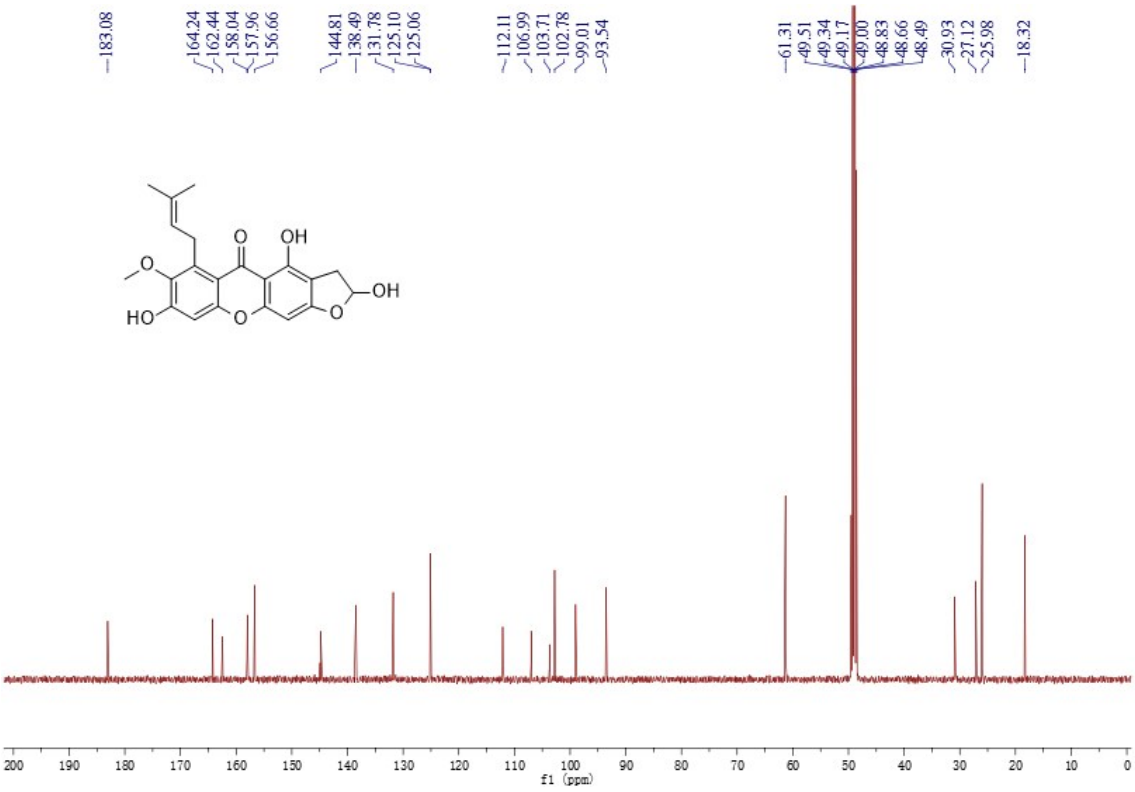


Figure 22S. ^{13}C NMR spectrum (CD_3OD, 125 MHz) of compound **2f**

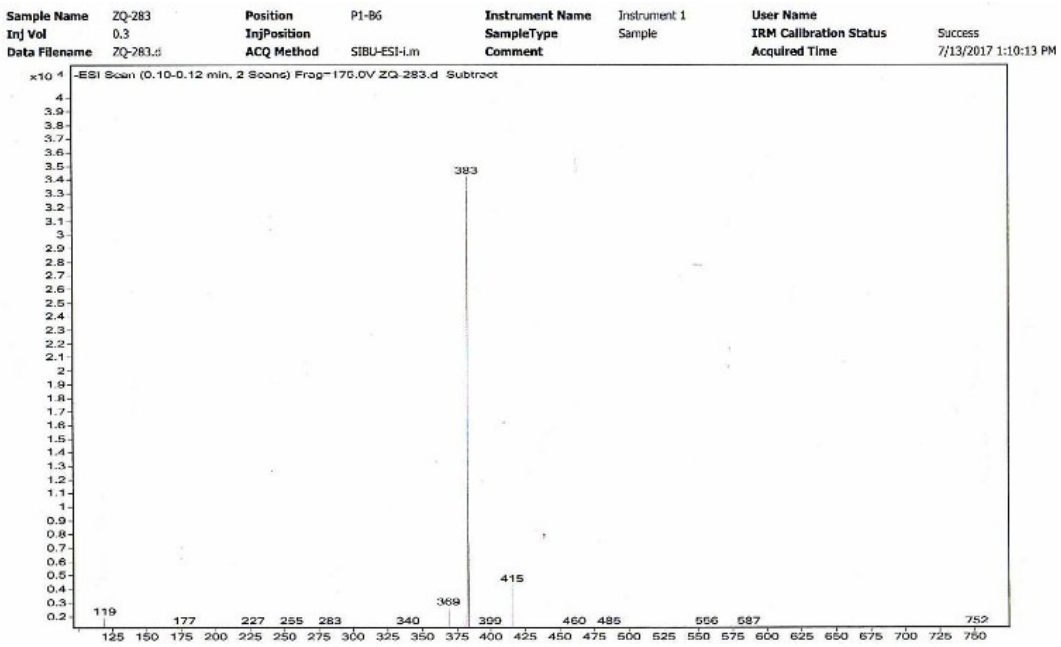


Figure 23S. Negative ESI-MS spectrum of compound **2f**

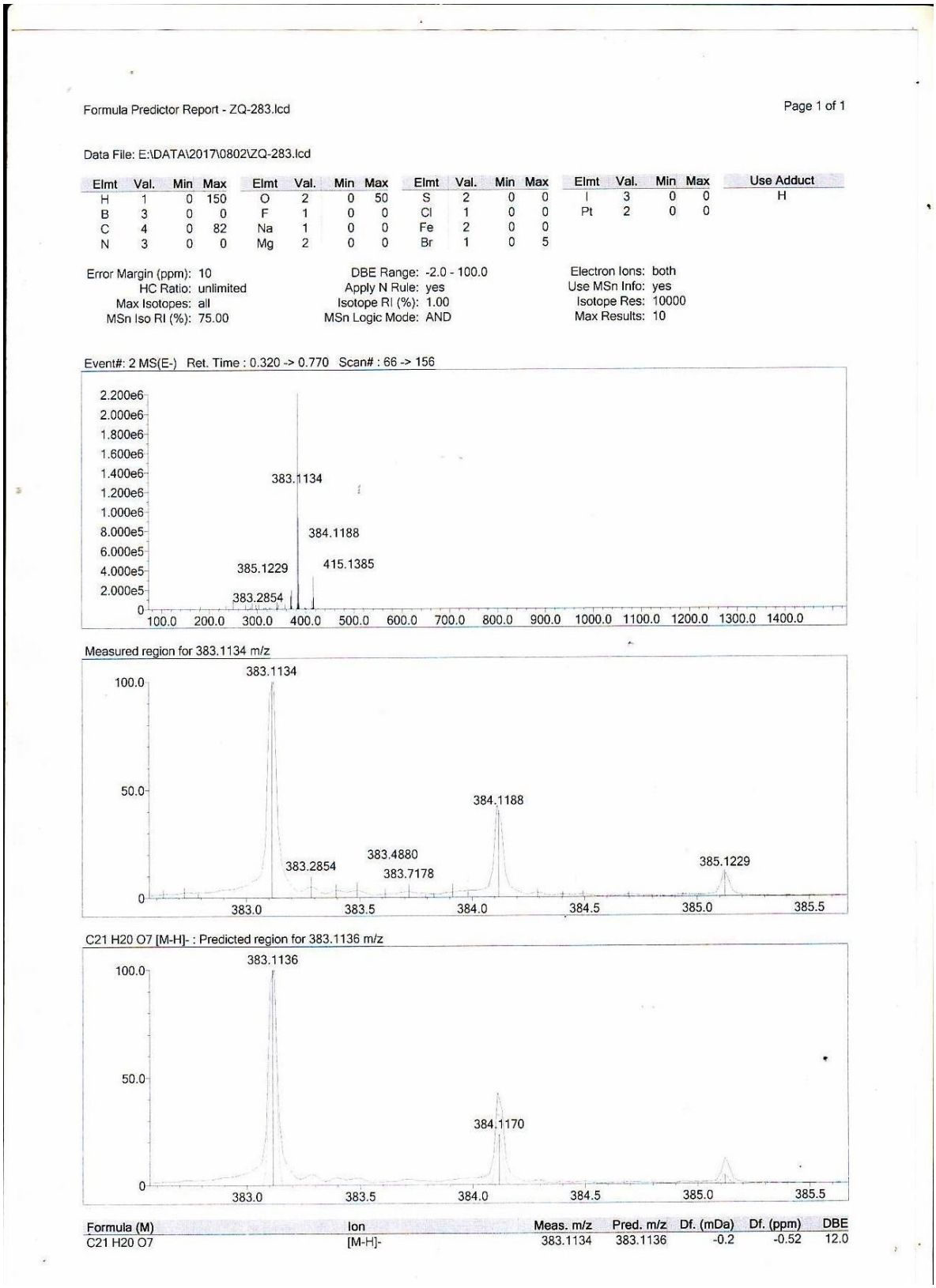


Figure 24S. Negative HR-ESIMS spectrum of compound **2f**

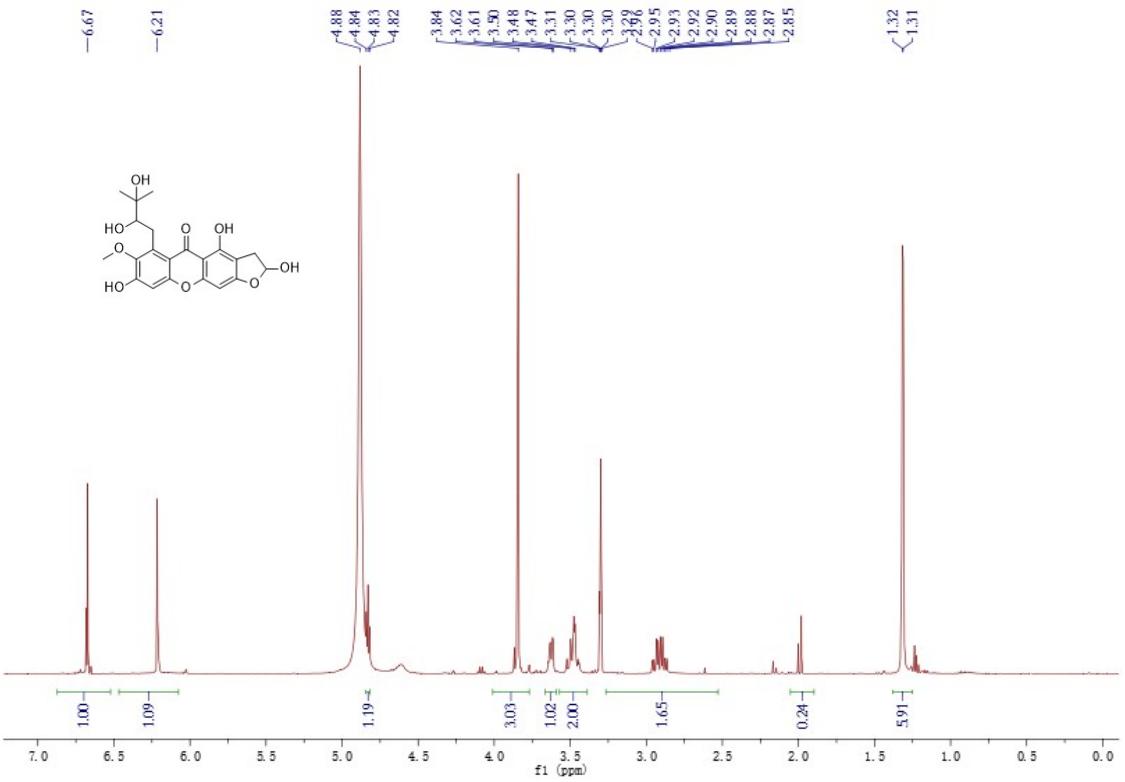


Figure 25S. ^{1}H NMR spectrum (CD_3OD, 500 MHz) of compound **2g**

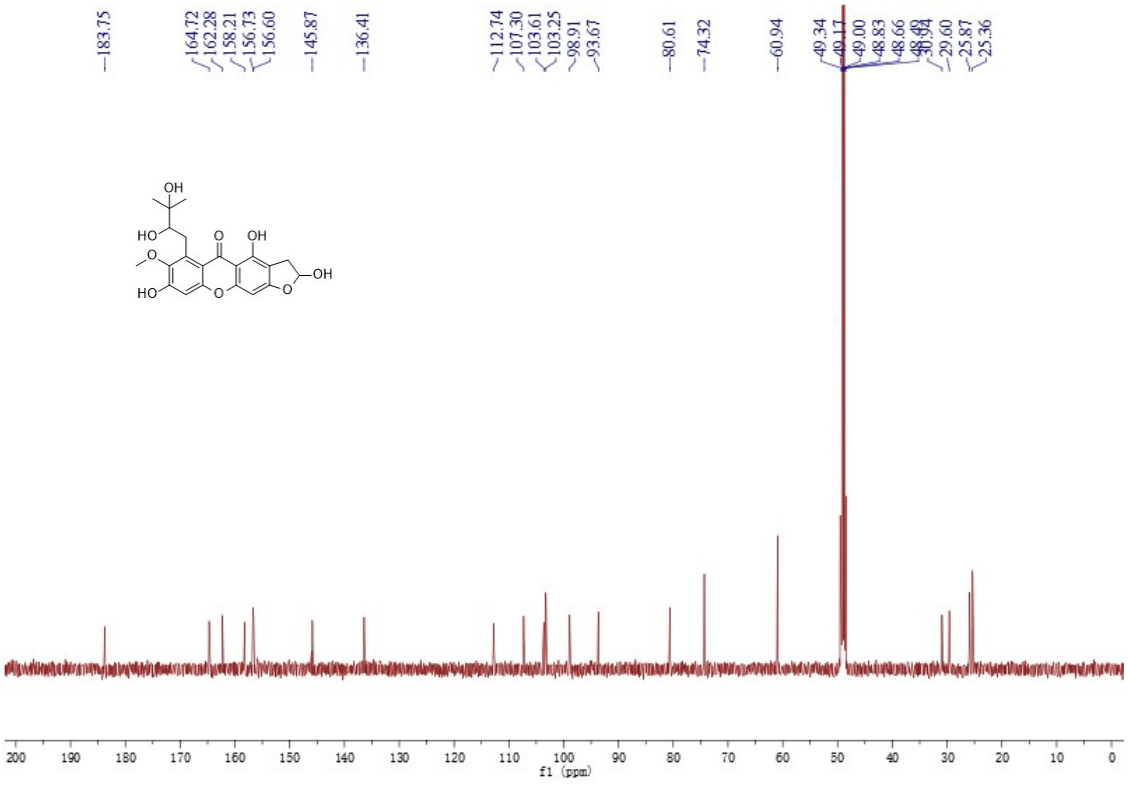


Figure 26S. ^{13}C NMR spectrum (CD_3OD, 125 MHz) of compound **2g**

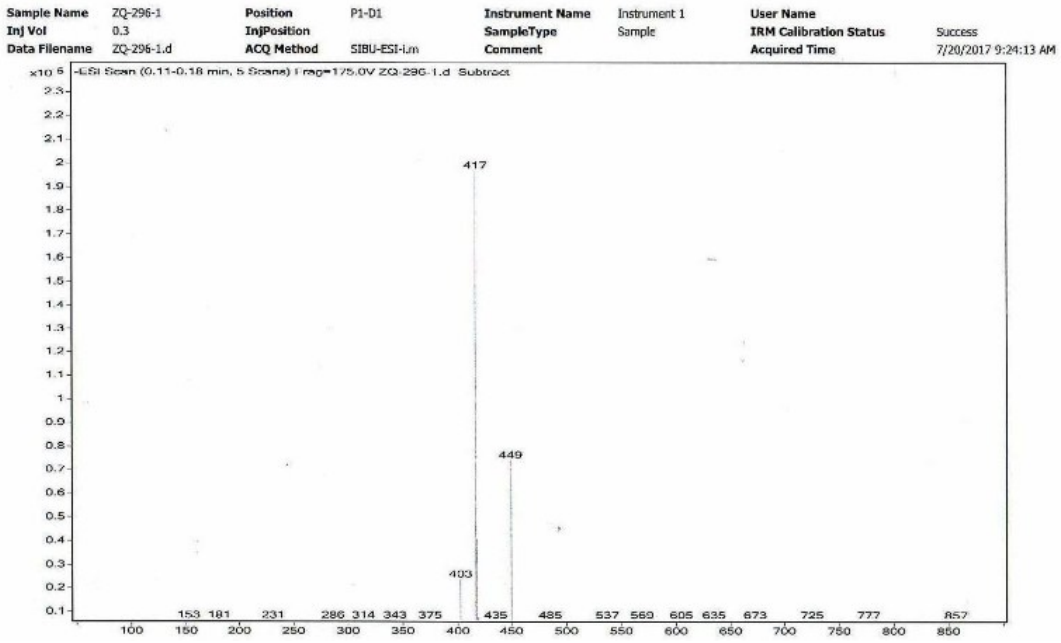


Figure 27S. Negative ESI-MS spectrum of compound **2g**

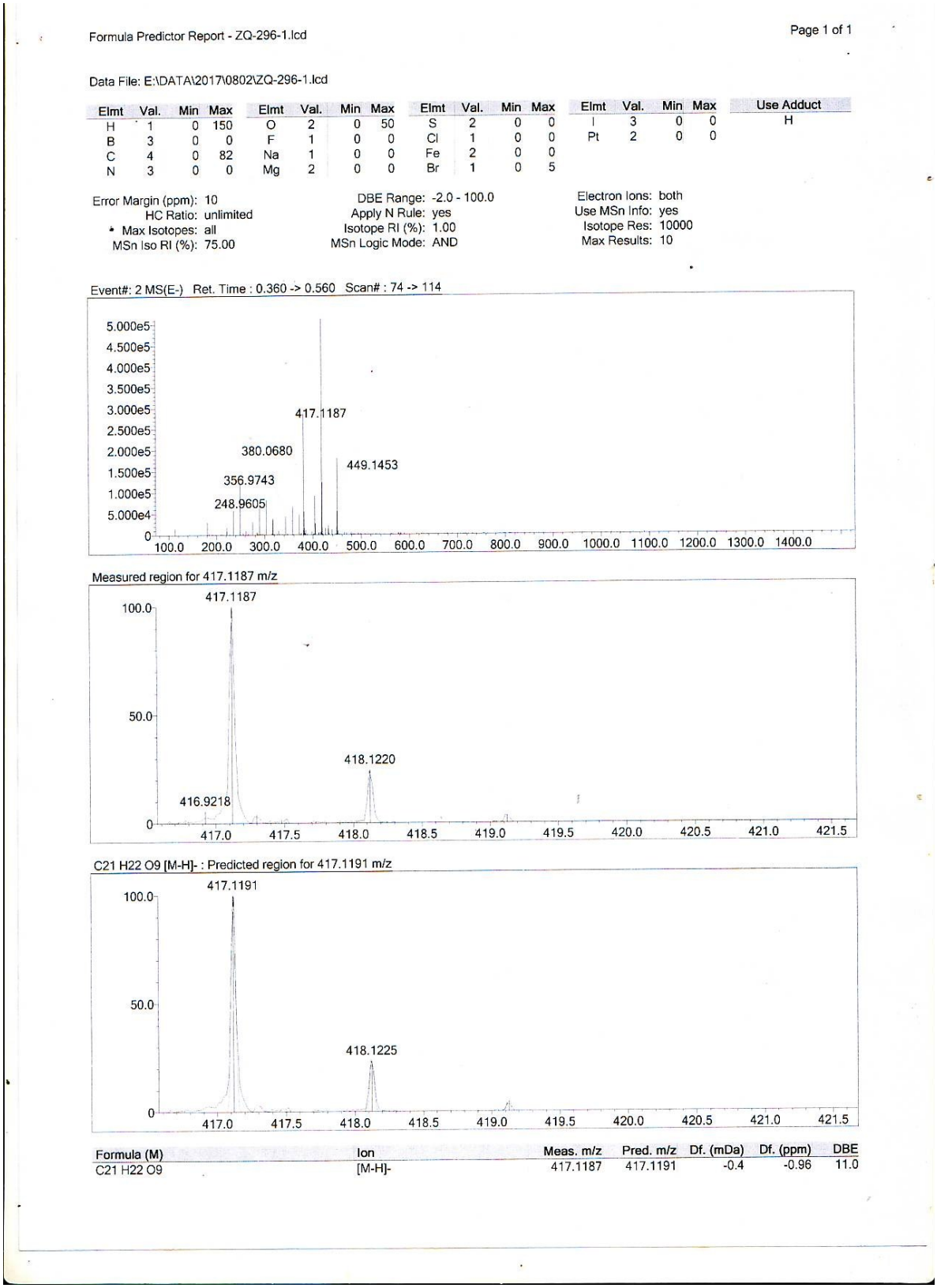


Figure 28S. Negative HR-ESIMS spectrum of compound **2g**

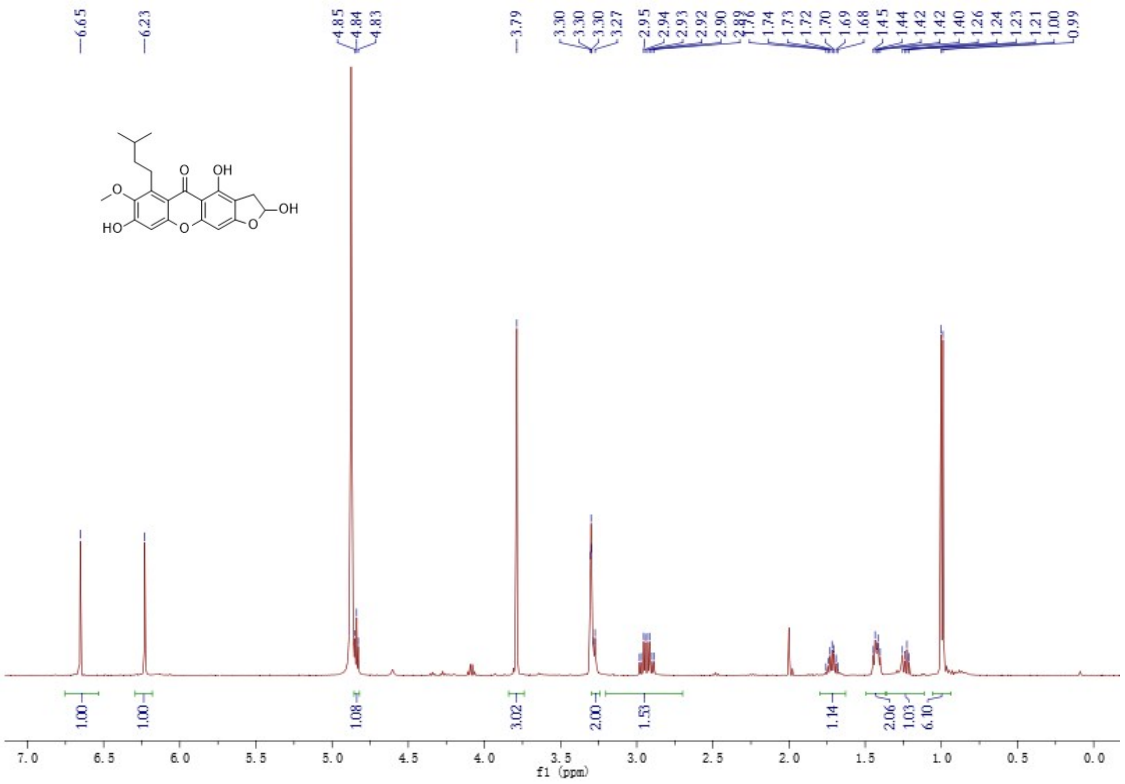


Figure 29S. ^{1}H NMR spectrum (CD_3OD, 500 MHz) of compound **2h**

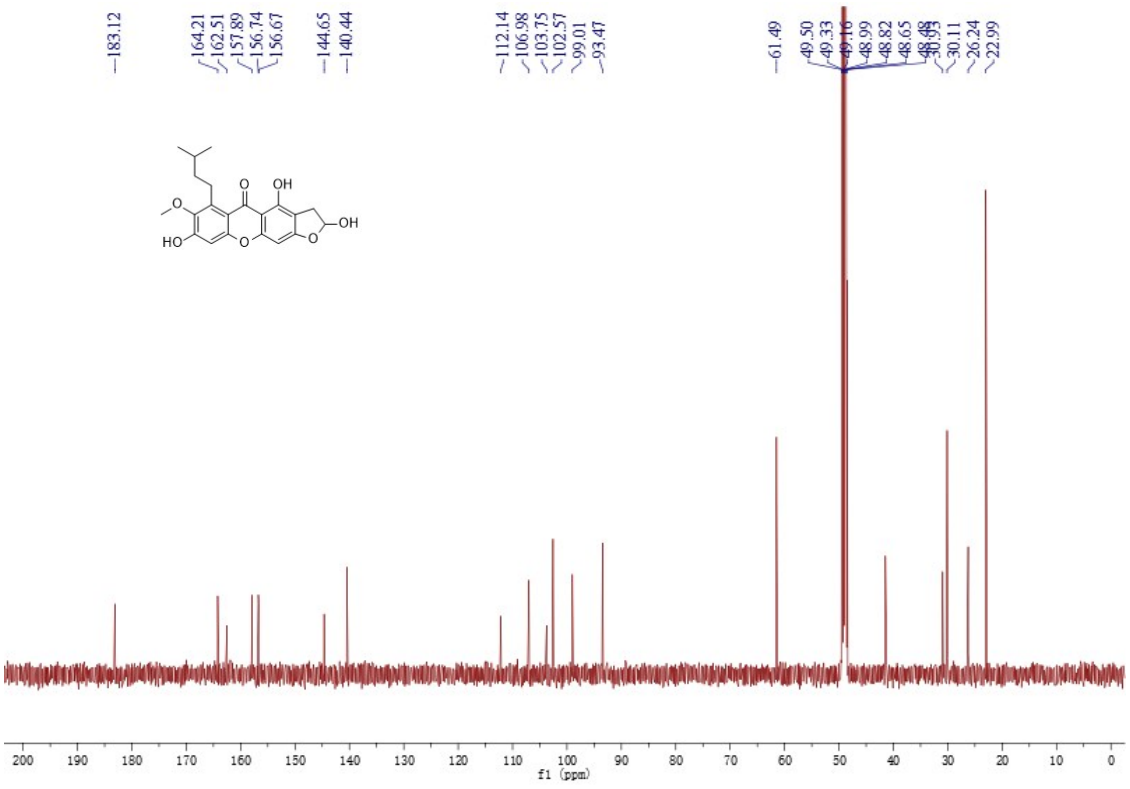


Figure 30S. ^{13}C NMR spectrum (CD_3OD, 125 MHz) of compound **2h**

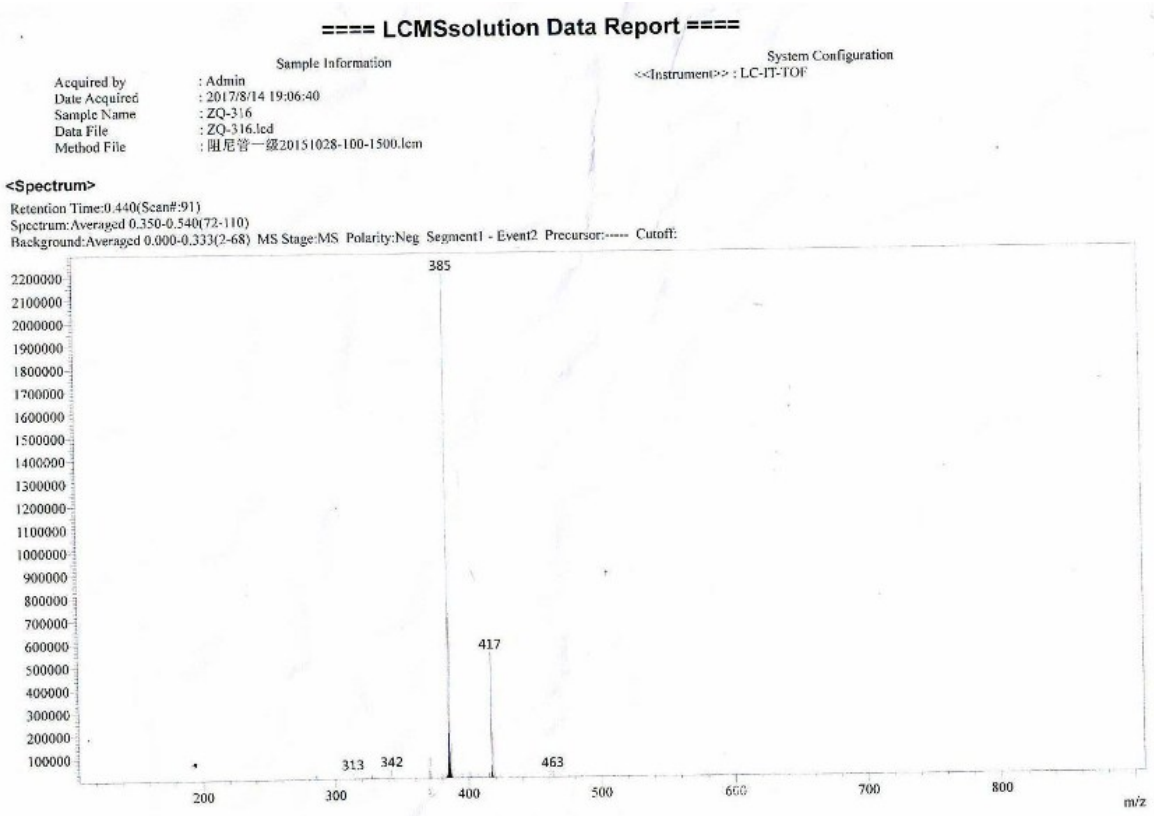


Figure 31S. Negative ESI-MS spectrum of compound **2h**

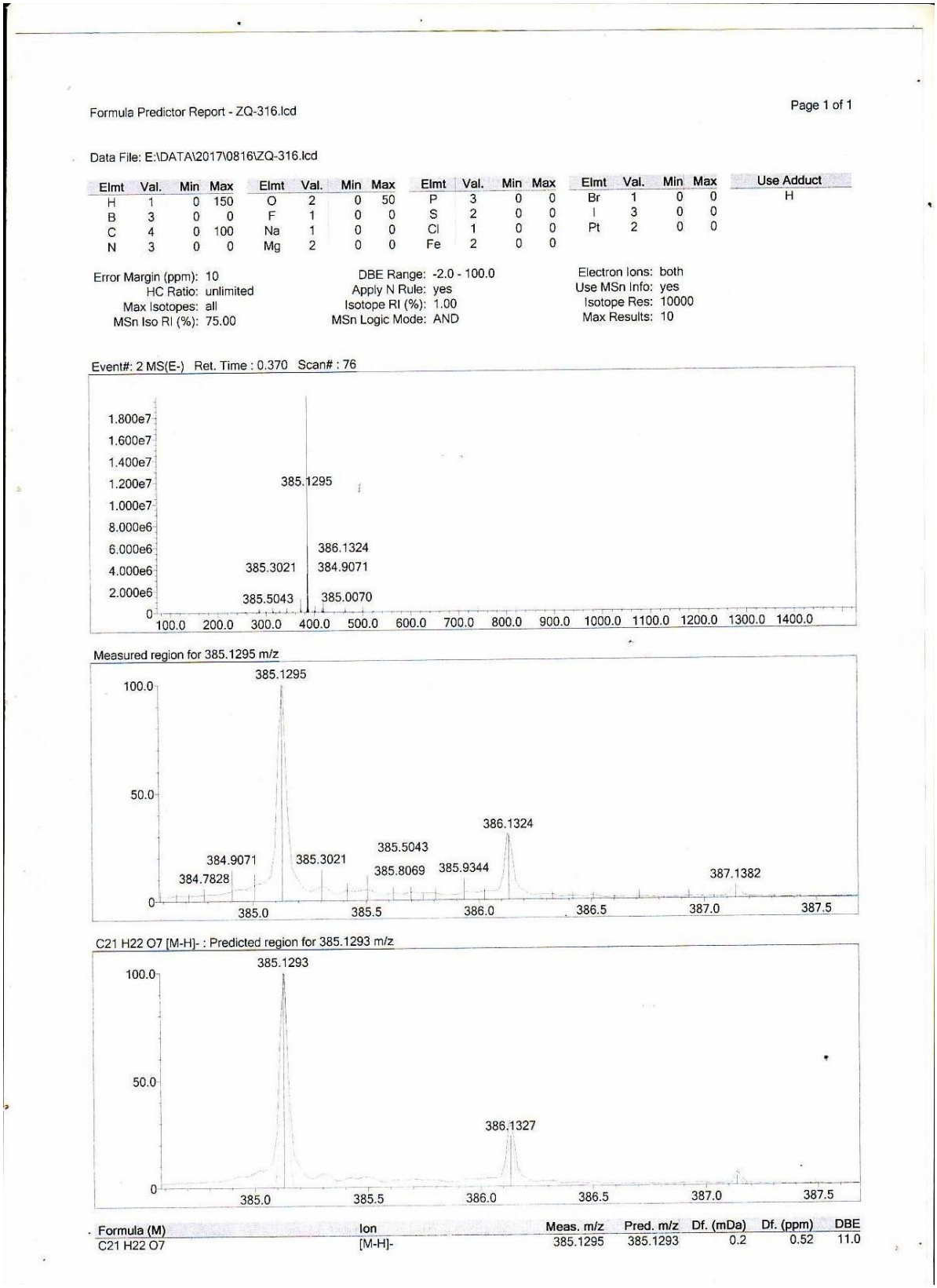


Figure 32S. Negative HR-ESIMS spectrum of compound **2h**

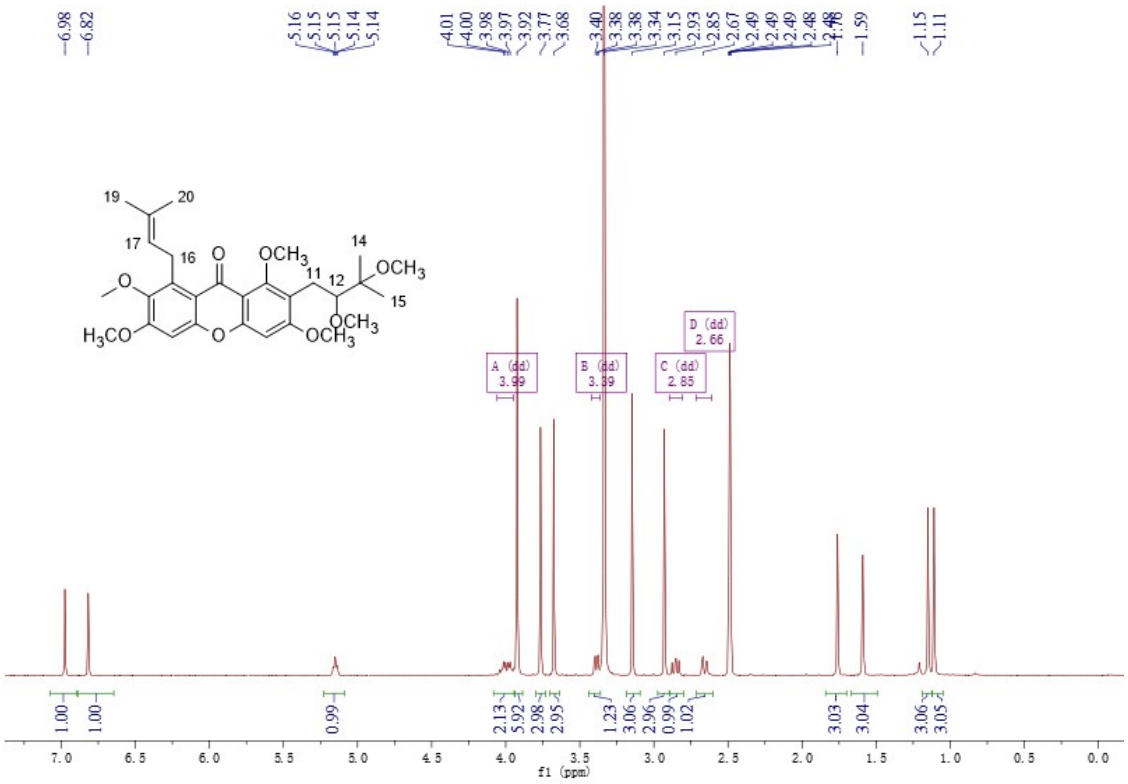


Figure 33S. ^{1}H NMR spectrum (DMSO-d_6, 500 MHz) of compound **2i**

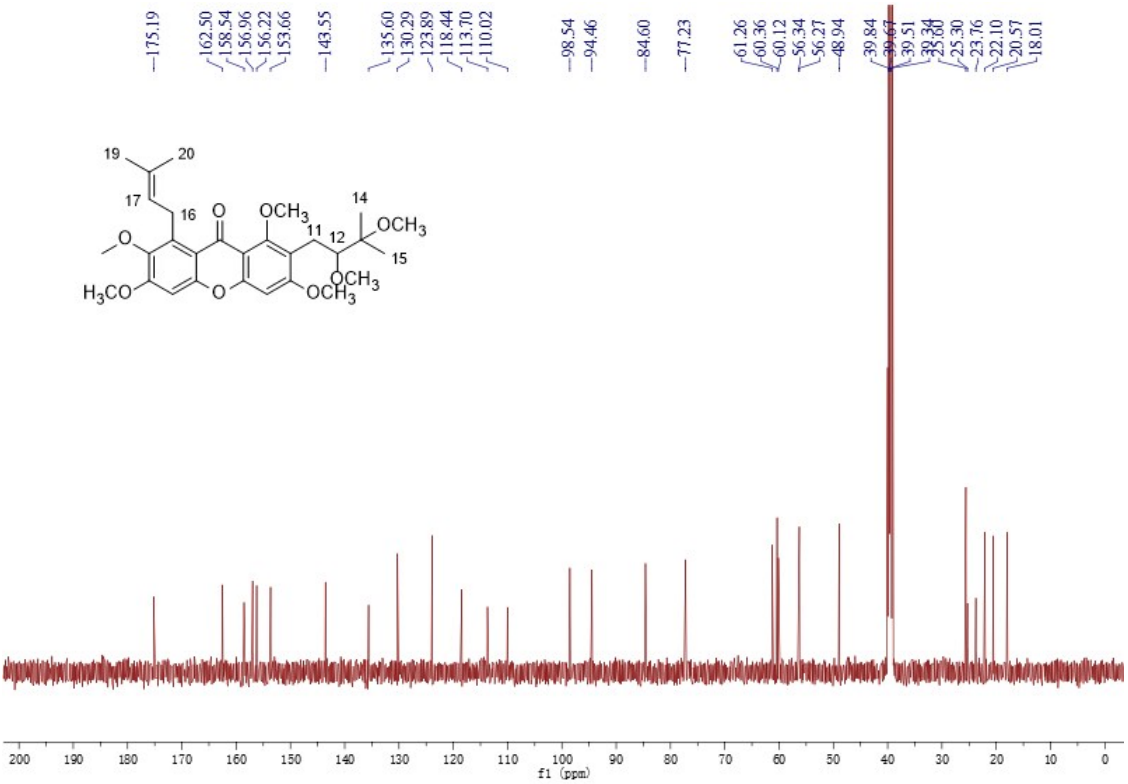


Figure 34S. ^{13}C NMR spectrum (DMSO-d_6, 125 MHz) of compound **2i**

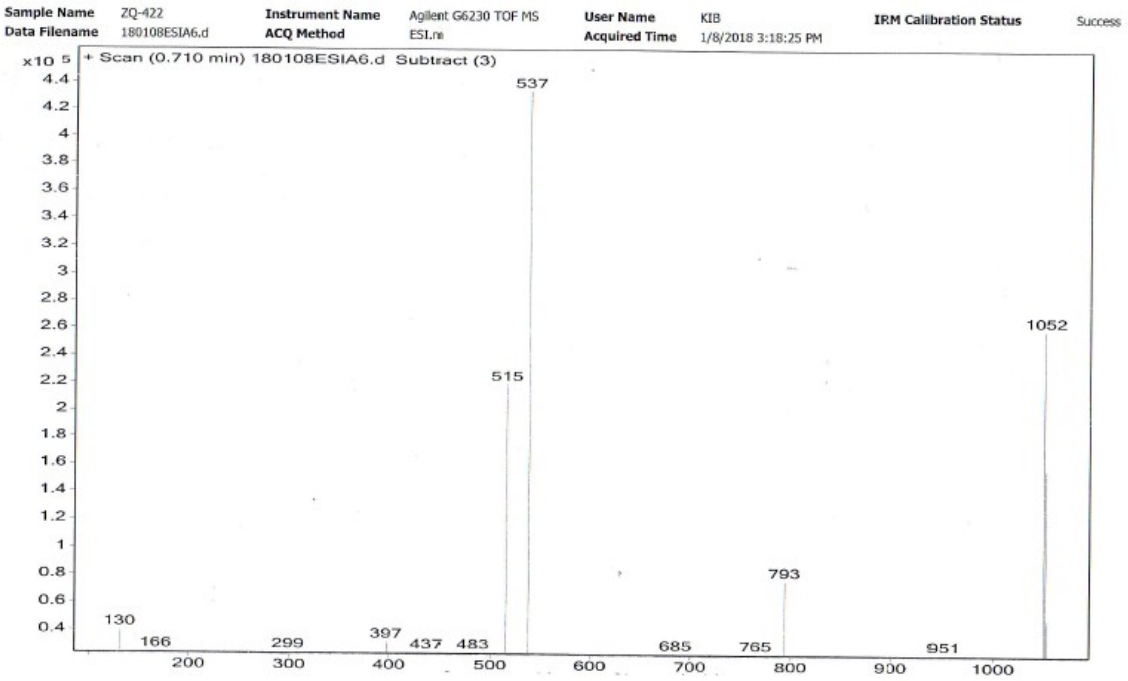
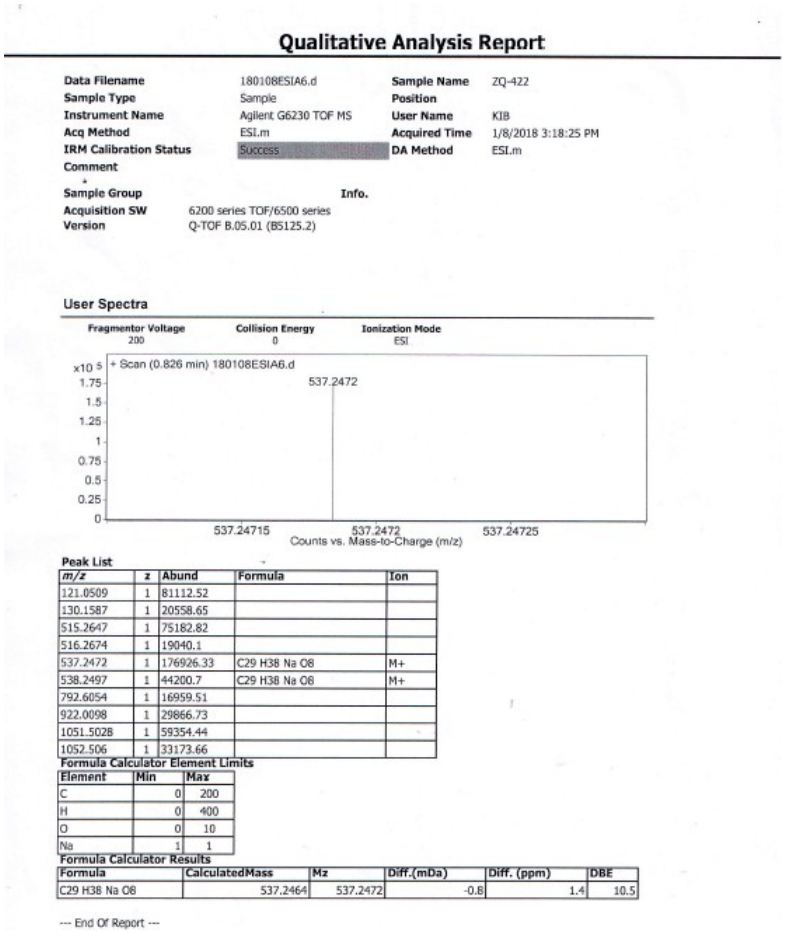


Figure 35S. Positive ESI-MS spectrum of compound **2i**



Qualitative Analysis Report

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Sample Type	Sample	**Position**	
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Acq Method	ESI.m	**Acquired Time**	1/8/2018 3:18:25 PM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)		

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI

Peak List

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515.2647	1	75182.82		
516.2674	1	19040.1		
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538.2497	1	44200.7	C29 H38 Na O8	M+
792.6054	1	16959.51		
922.0098	1	29866.73		
1051.5028	1	59354.44		
1052.506	1	33173.66		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	0	10
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
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--- End Of Report ---

Figure 36S. Positive HR-ESIMS spectrum of compound **2i**

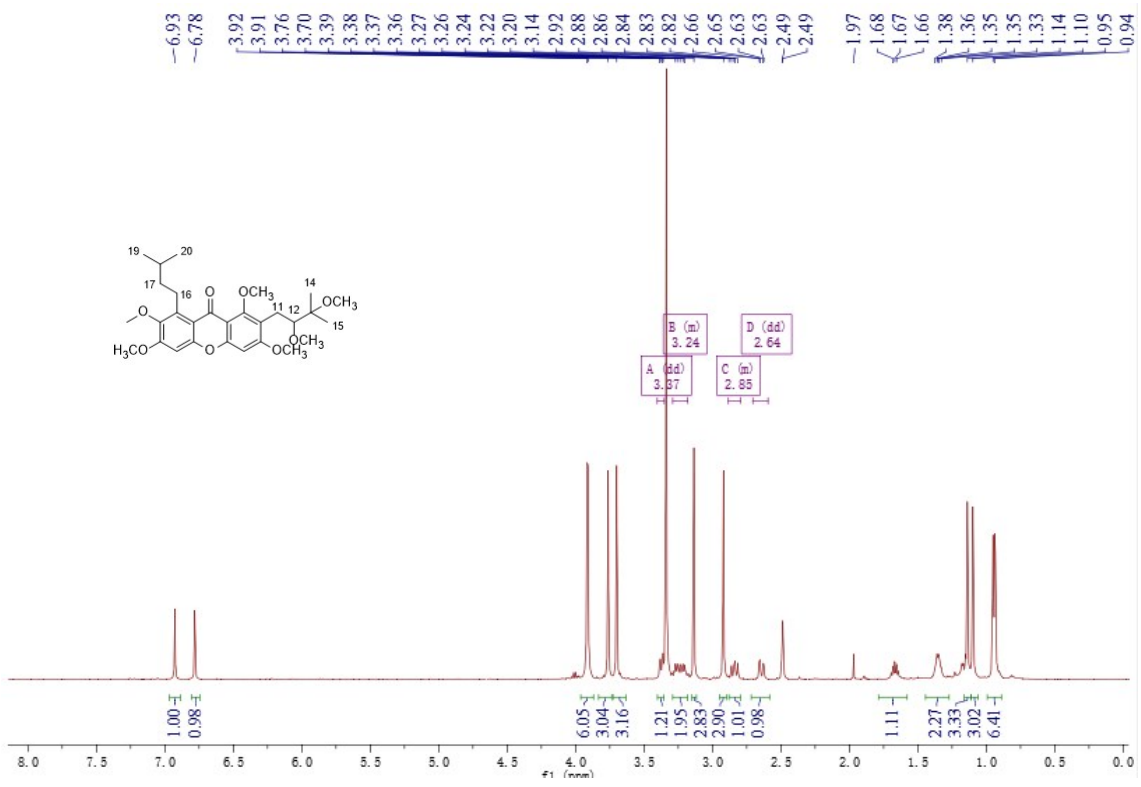


Figure 37S. [1]H NMR spectrum (DMSO-d_6, 500 MHz) of compound **2j**

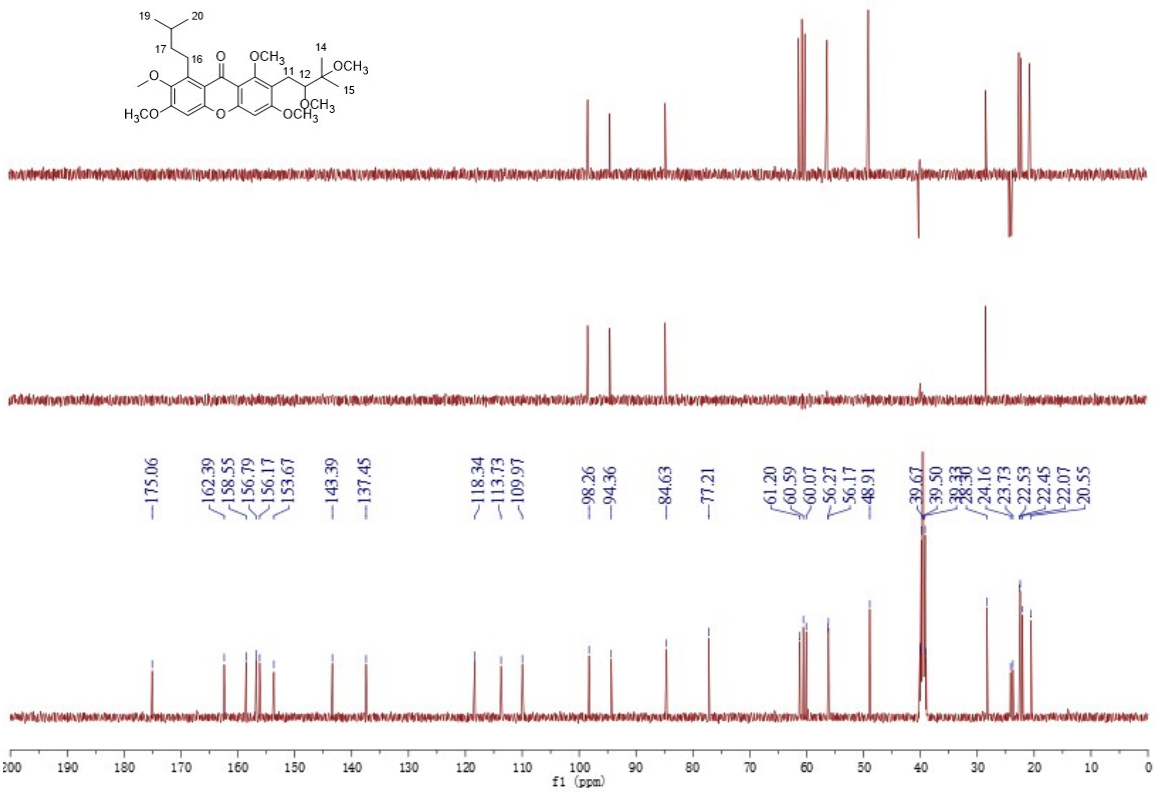


Figure 38S. [13]C NMR spectrum (DMSO-d_6, 125 MHz) of compound **2j**

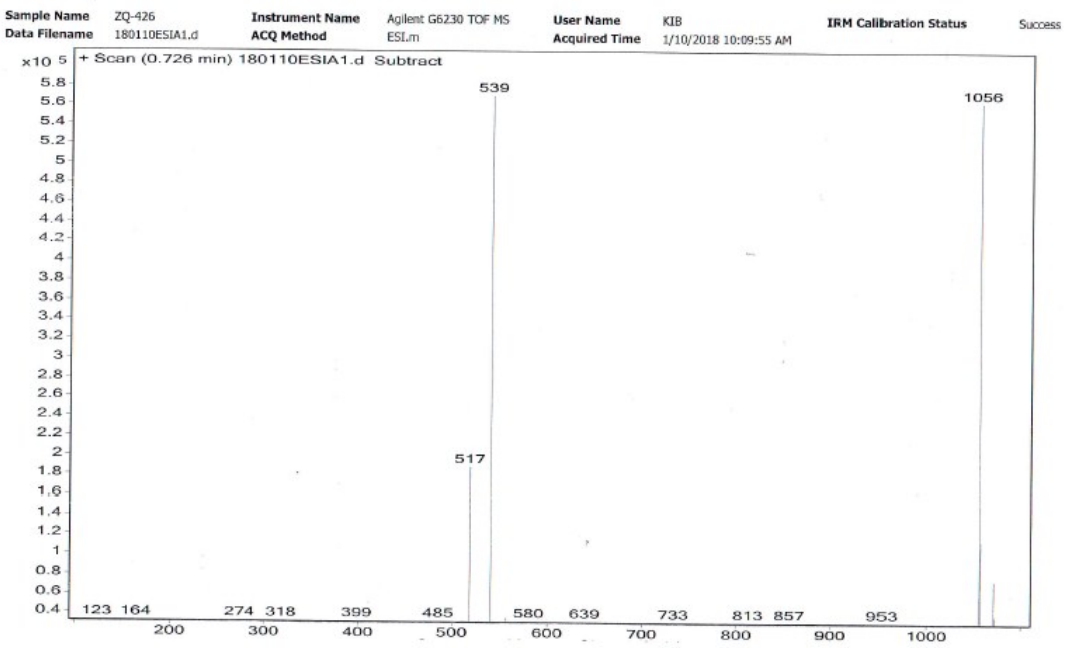
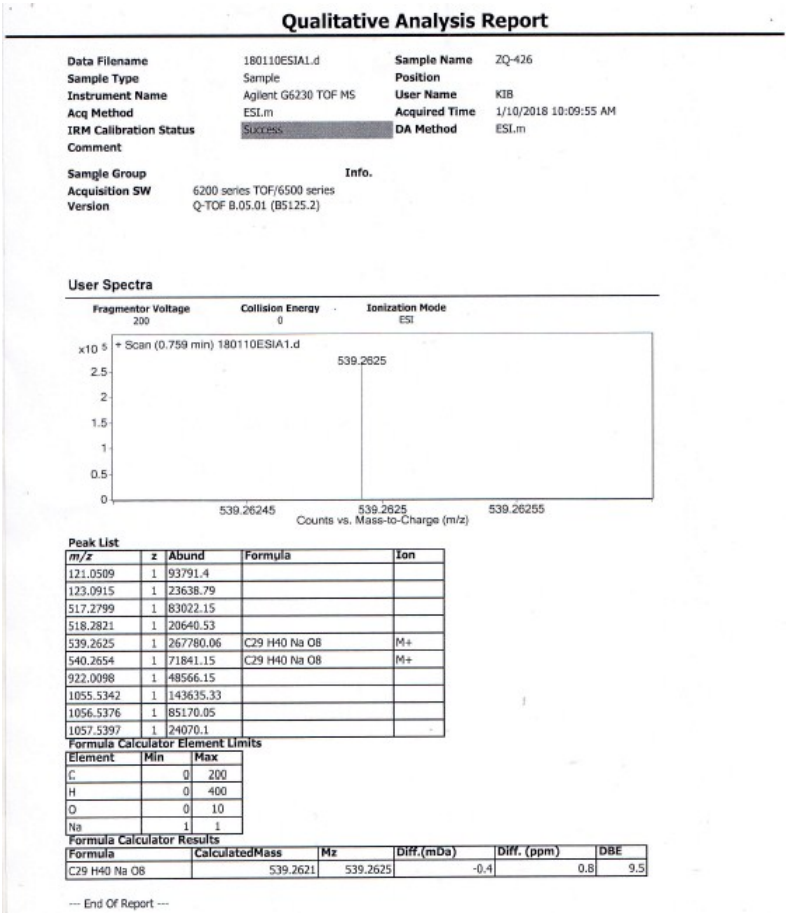


Figure 39S. Positive ESI-MS spectrum of compound **2j**



Qualitative Analysis Report

Data Filename	180110ESIA1.d	Sample Name	ZQ-426
Sample Type	Sample	Position	
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Acq Method	ESI.m	Acquired Time	1/10/2018 10:09:55 AM
IRM Calibration Status	Success	DA Method	ESI.m
Comment			
Sample Group		Info.	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)		

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI

+ Scan (0.759 min) 180110ESIA1.d

539.2625

539.26245 539.2625 539.26255

Counts vs. Mass-to-Charge (m/z)

Peak List

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123.0915	1	23638.79		
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518.2821	1	20640.53		
539.2625	1	267780.06	C29 H40 Na O8	M+
540.2654	1	71841.15	C29 H40 Na O8	M+
922.0098	1	48566.15		
1055.5342	1	143635.33		
1056.5376	1	85170.05		
1057.5397	1	24070.1		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	0	10
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
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--- End Of Report ---

Figure 40S. Positive HR-ESIMS spectrum of compound **2j**

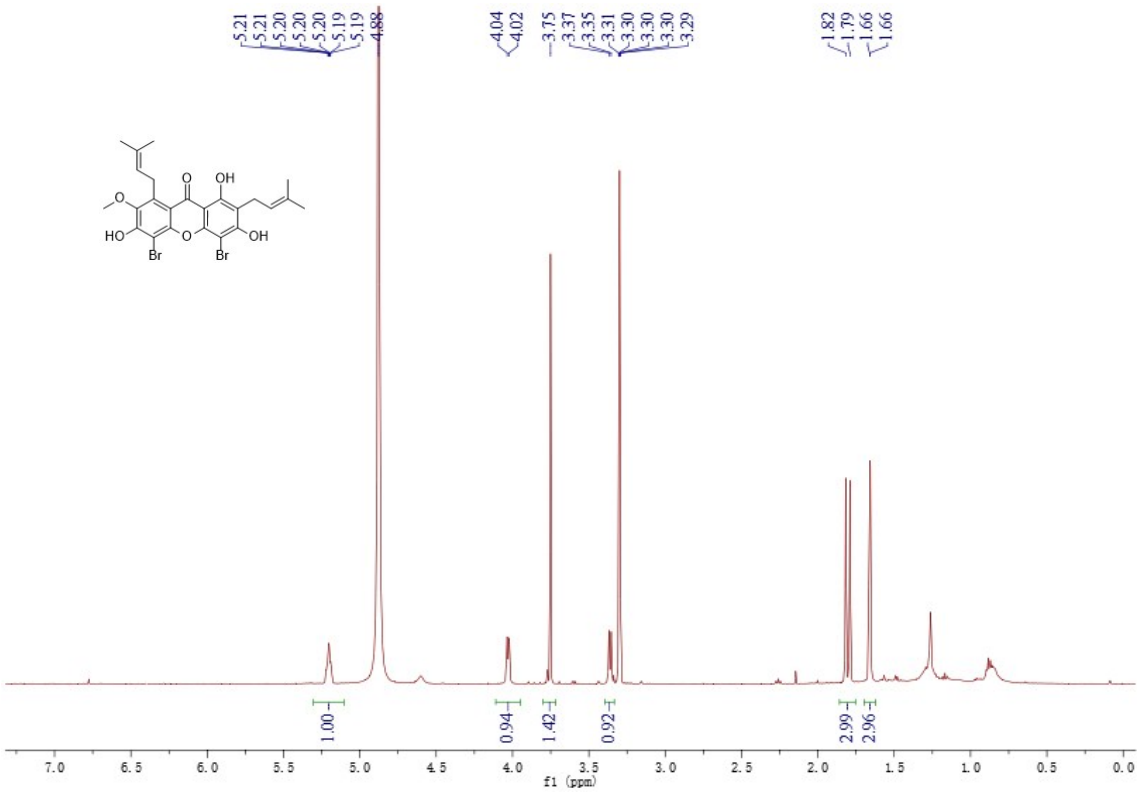


Figure 41S. ^{1}H NMR spectrum (CD_3OD, 500 MHz) of compound **3c**

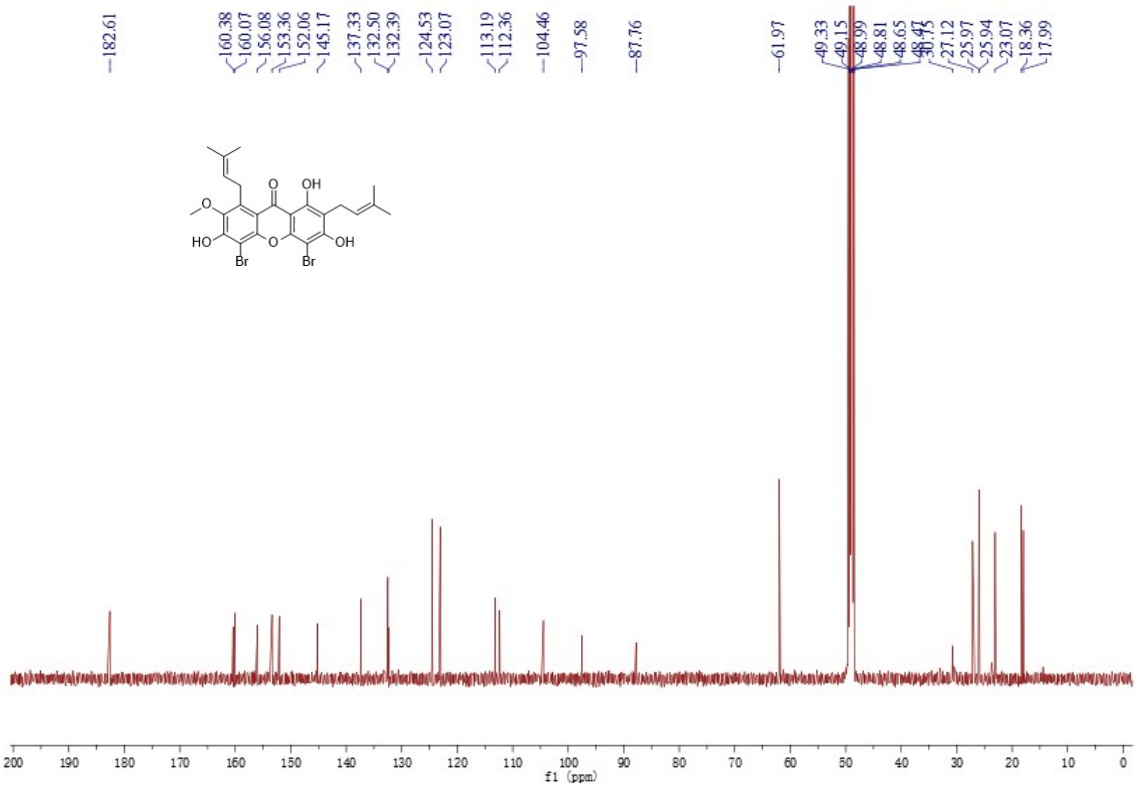


Figure 42S. ^{13}C NMR spectrum (CD_3OD, 125 MHz) of compound **3c**

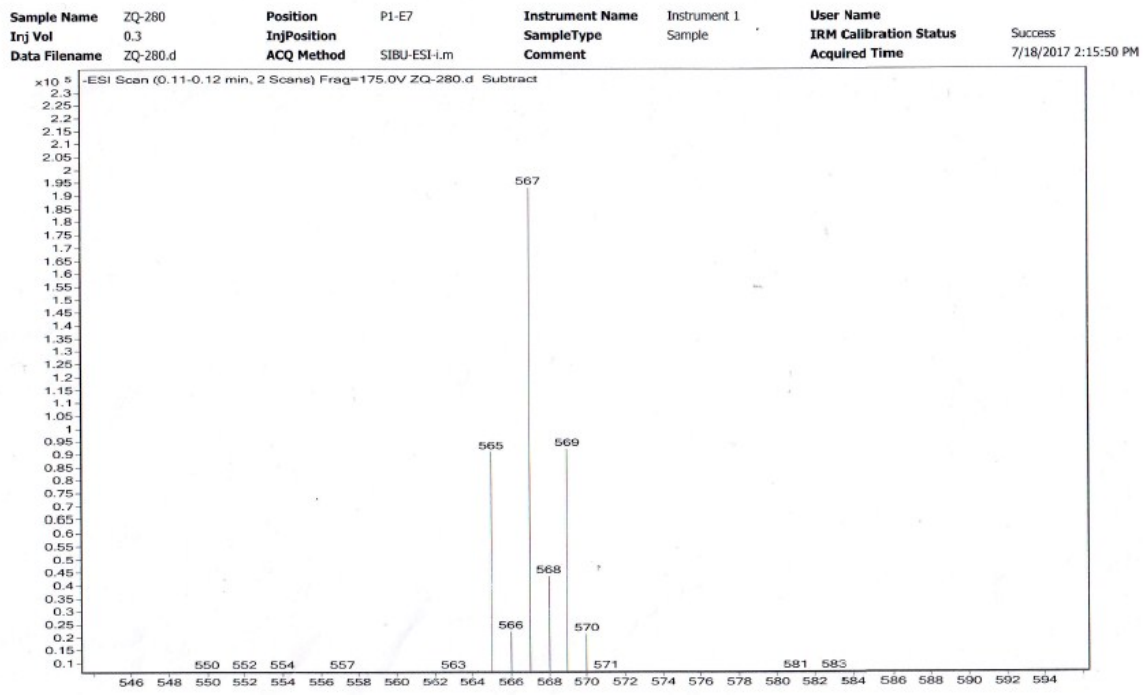


Figure 43S. Negative ESI-MS spectrum of compound **3c**

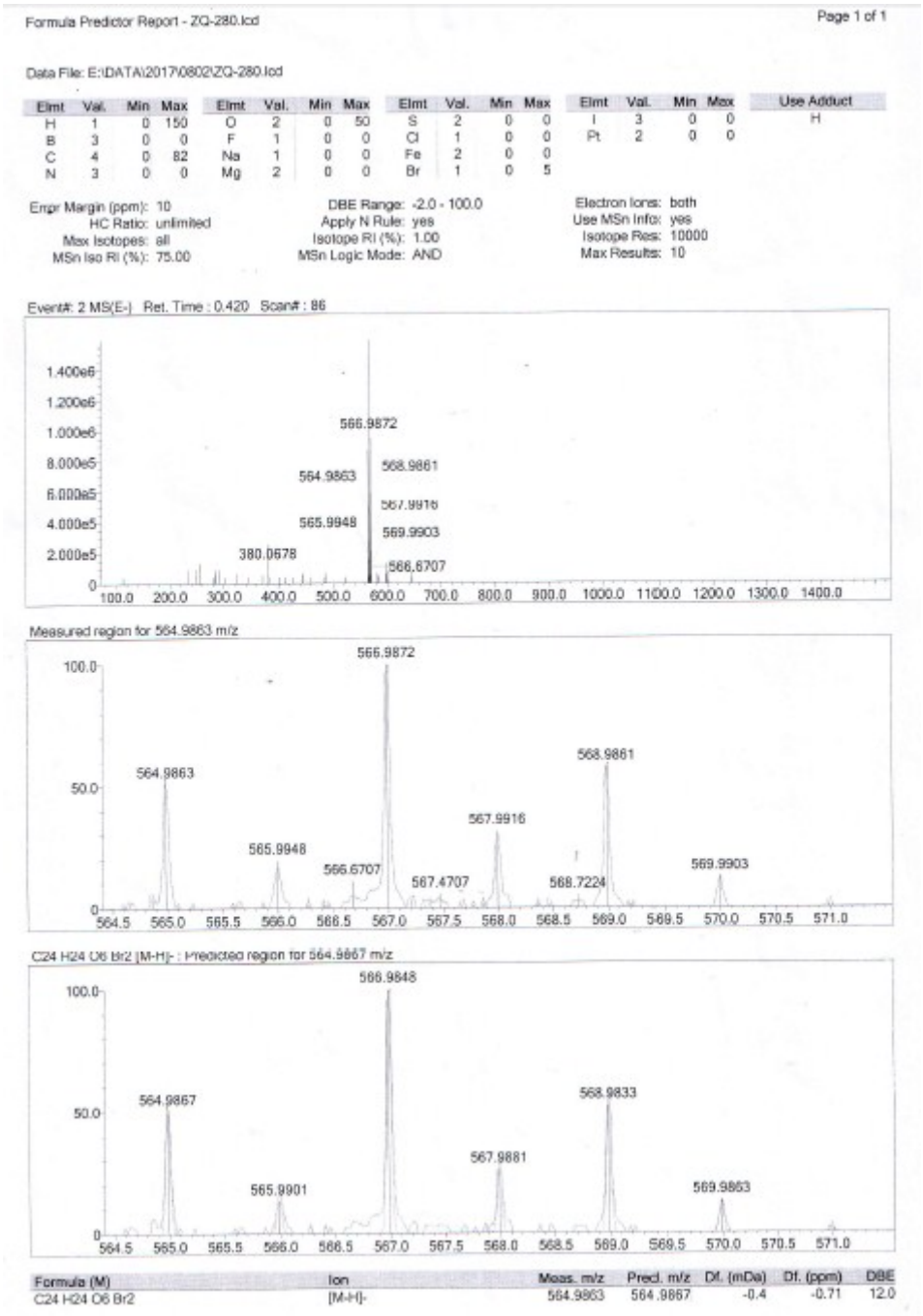


Figure 44S. Negative HR-ESIMS spectrum of compound **3c**

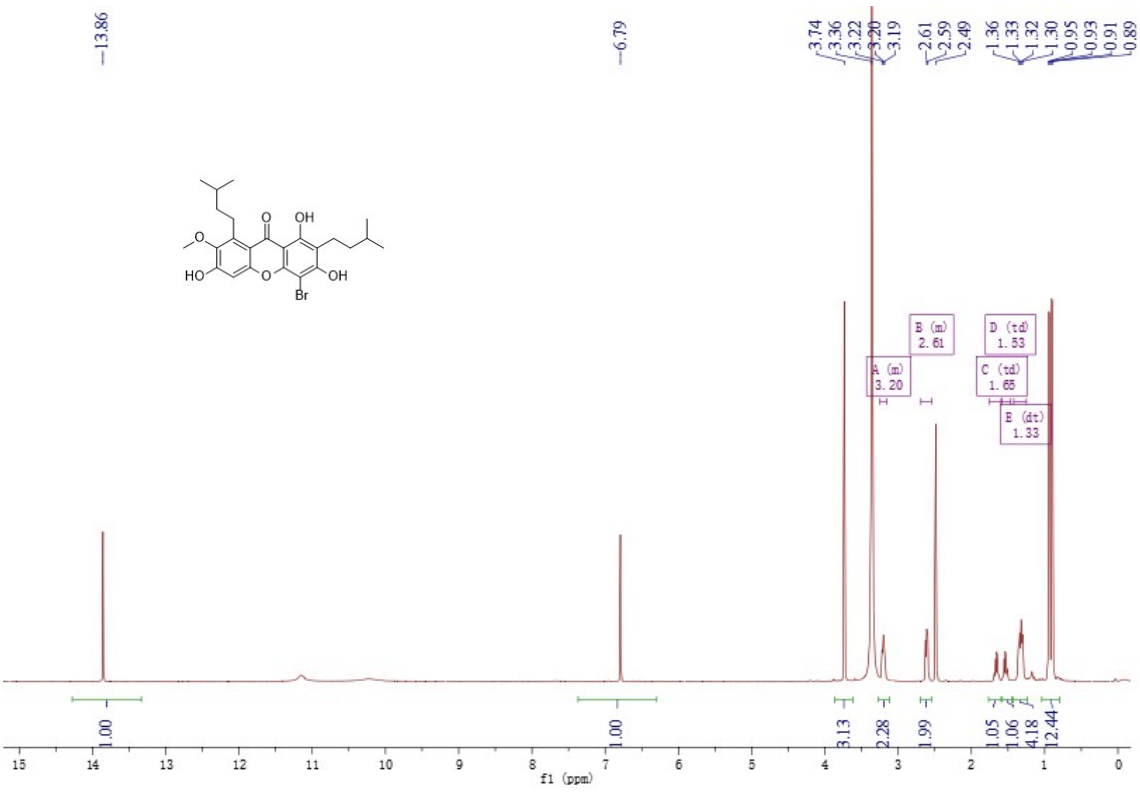


Figure 45S. [1]H NMR spectrum (DMSO-d_6, 500 MHz) of compound **3d**

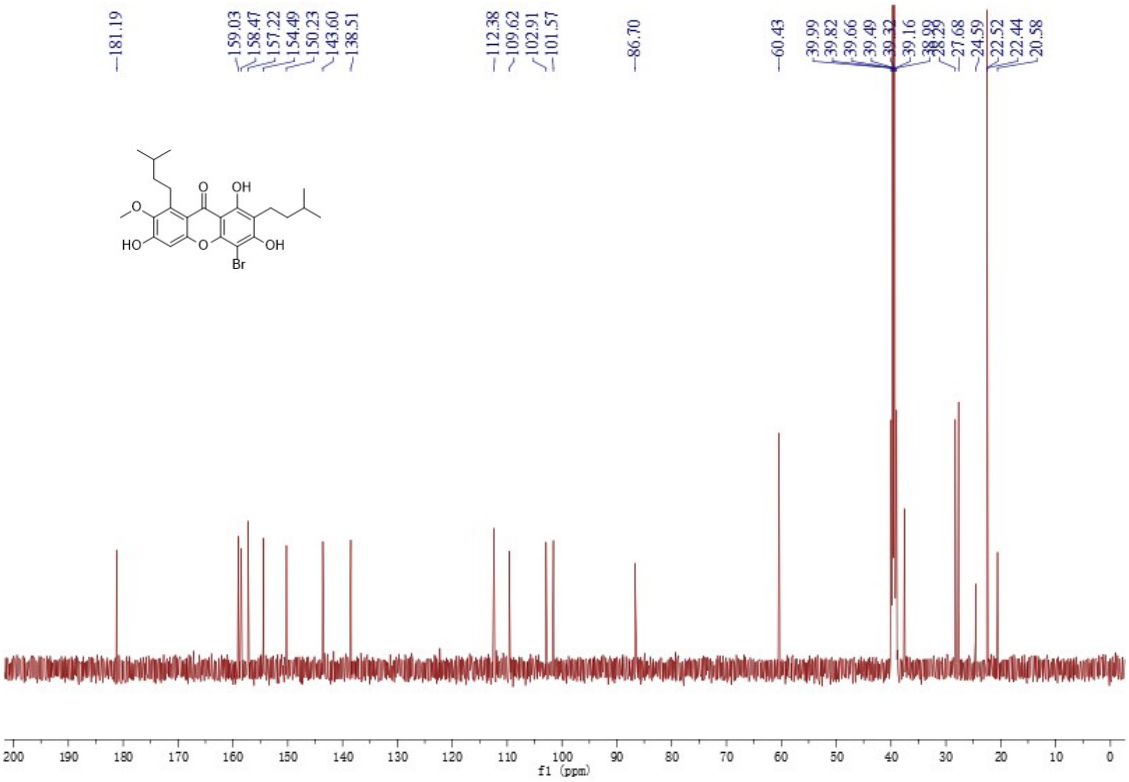


Figure 46S. [13]C NMR spectrum (DMSO-d_6, 125 MHz) of compound **3d**

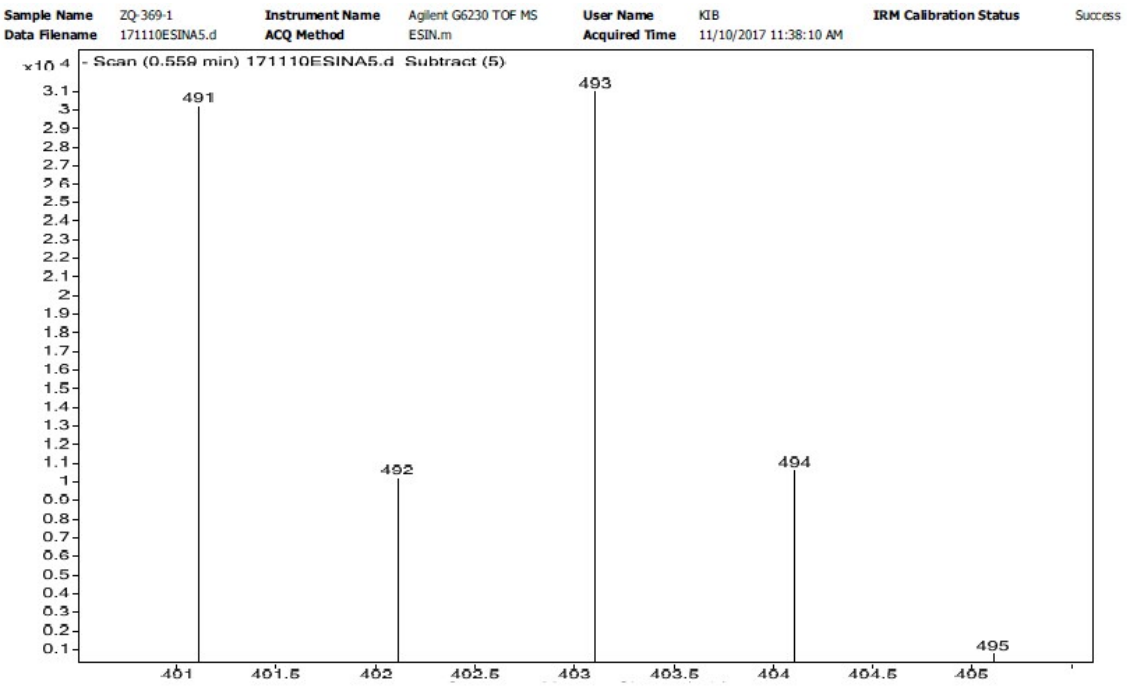
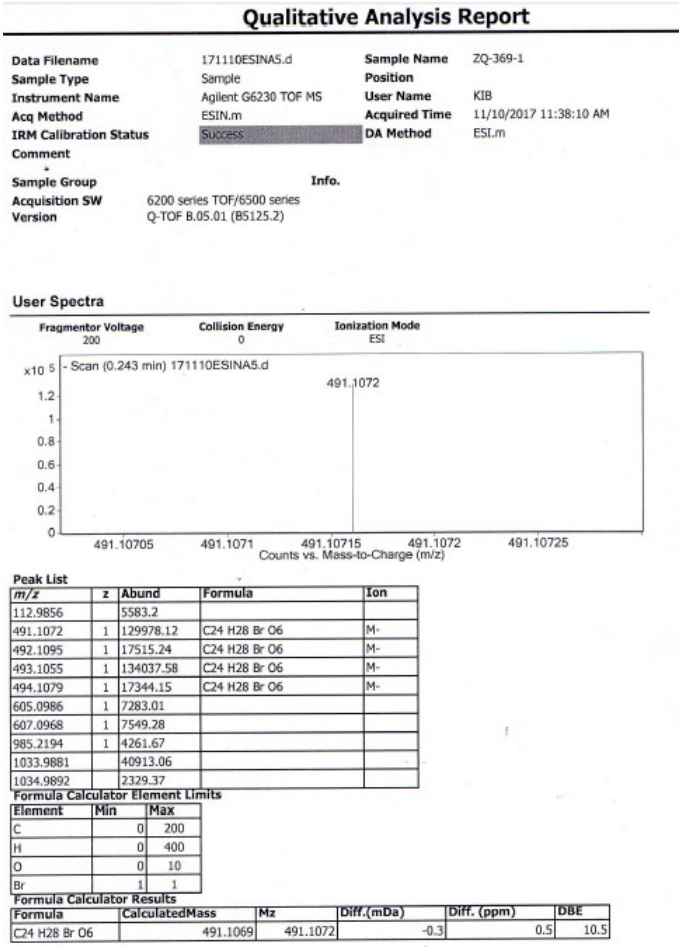


Figure 47S. Negative ESI-MS spectrum of compound **3d**



Qualitative Analysis Report

Data Filename	171110ESINA5.d	Sample Name	ZQ-369-1
Sample Type	Sample	Position	
Instrument Name	Agilent G6230 TOF MS	User Name	KIB
Acq Method	ESIN.m	Acquired Time	11/10/2017 11:38:10 AM
IRM Calibration Status	Success	DA Method	ESI.m
Comment			
Sample Group		Info.	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)		

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI

Peak List

m/z	z	Abund	Formula	Ion
112.9856		5583.2		
491.1072	1	129978.12	C24 H28 Br O6	M-
492.1095	1	17515.24	C24 H28 Br O6	M-
493.1055	1	134037.58	C24 H28 Br O6	M-
494.1079	1	17344.15	C24 H28 Br O6	M-
605.0986	1	7283.01		
607.0968	1	7549.28		
985.2194	1	4261.67		
1033.9881		40913.06		
1034.9892		2329.37		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	0	10
Br	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C24 H28 Br O6	491.1069	491.1072	-0.3	0.5	10.5

Figure 48S. Negative HR-ESIMS spectrum of compound **3d**

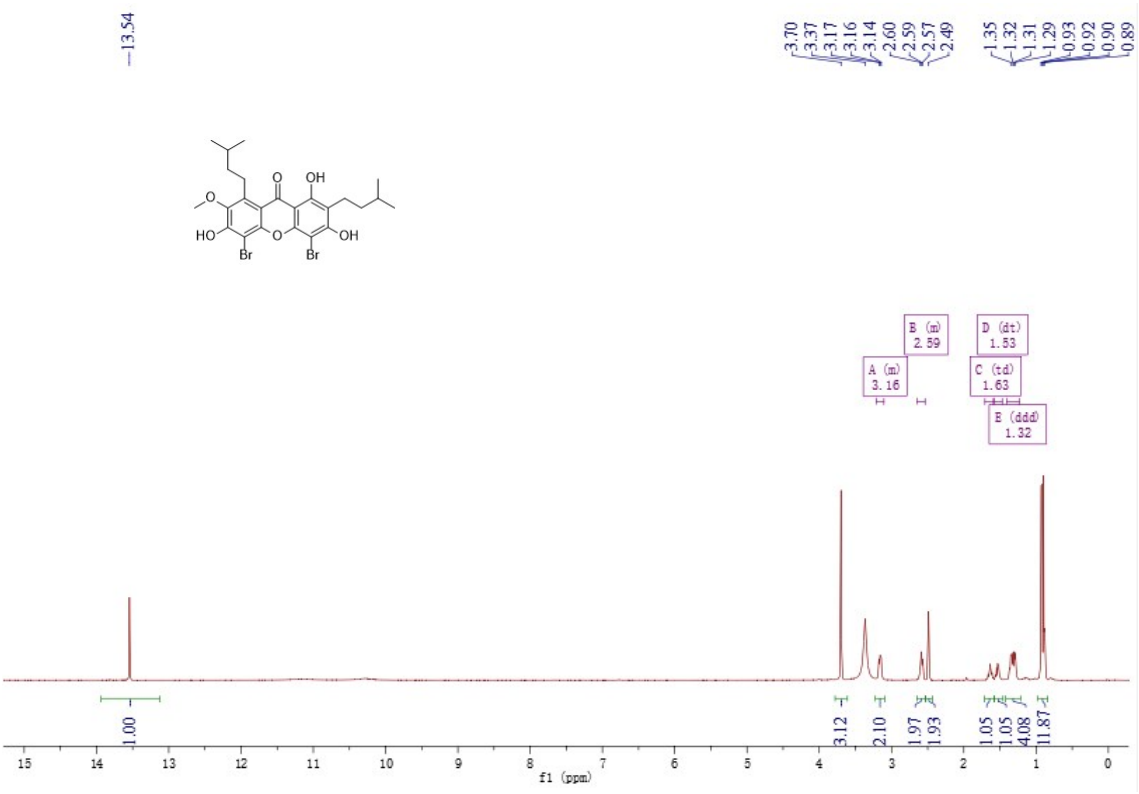


Figure 49S. [1]H NMR spectrum (DMSO-d_6, 500 MHz) of compound **3e**

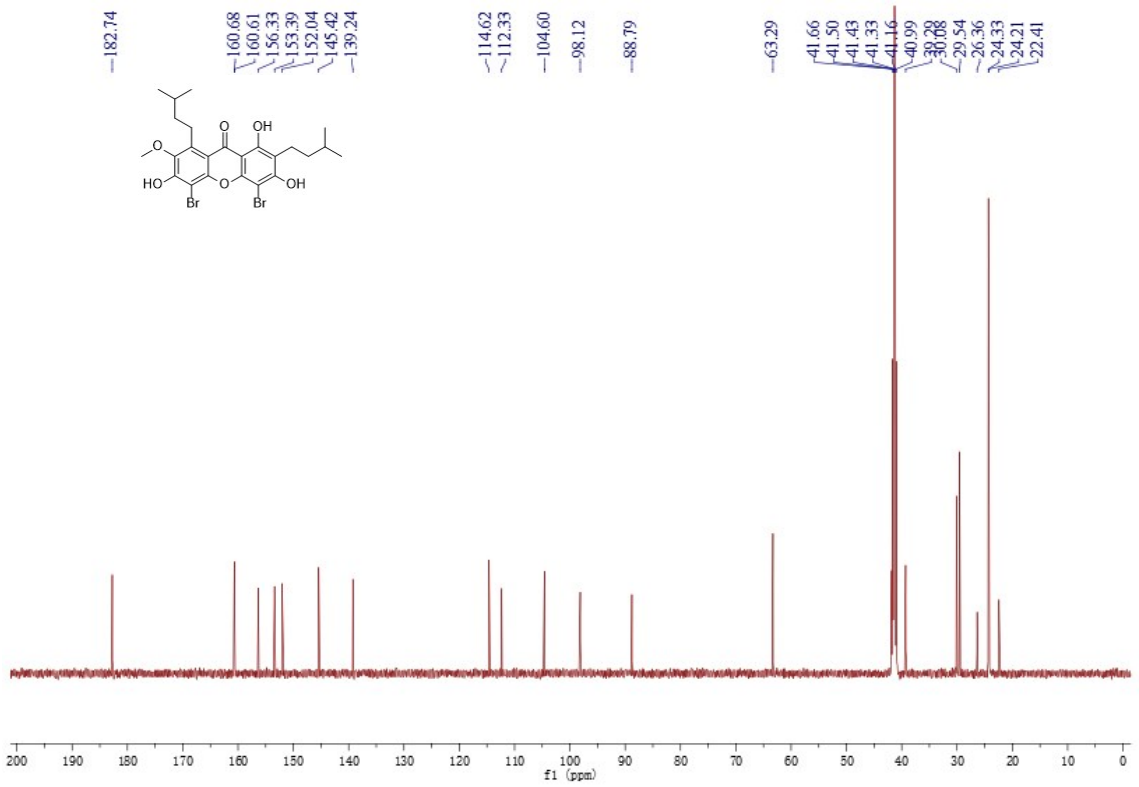


Figure 50S. [13]C NMR spectrum (DMSO-d_6, 125 MHz) of compound **3e**

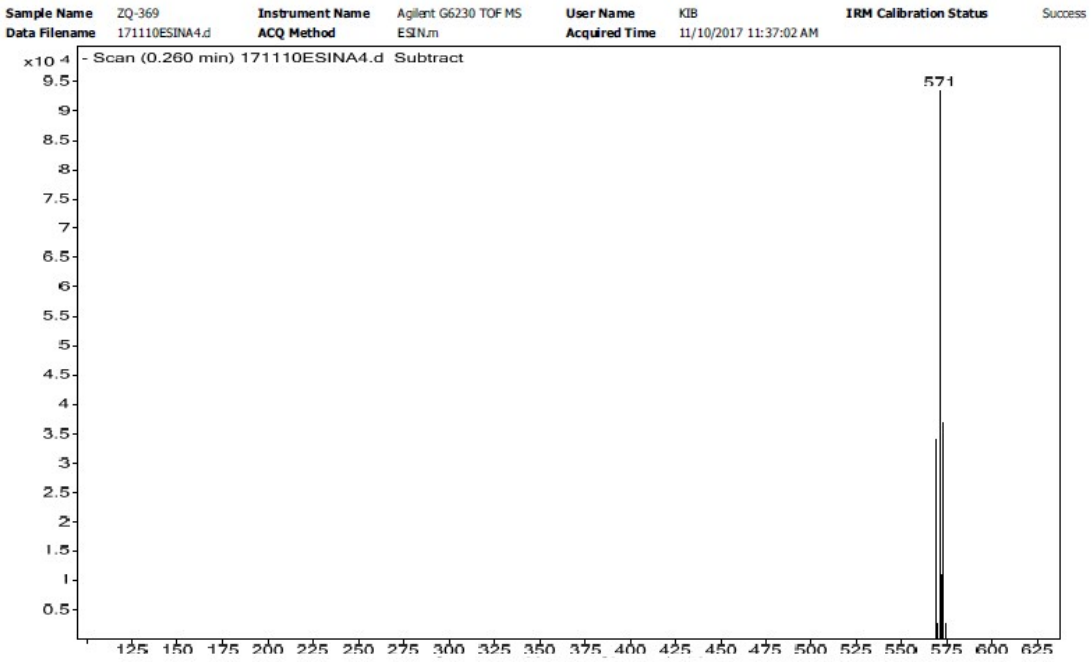
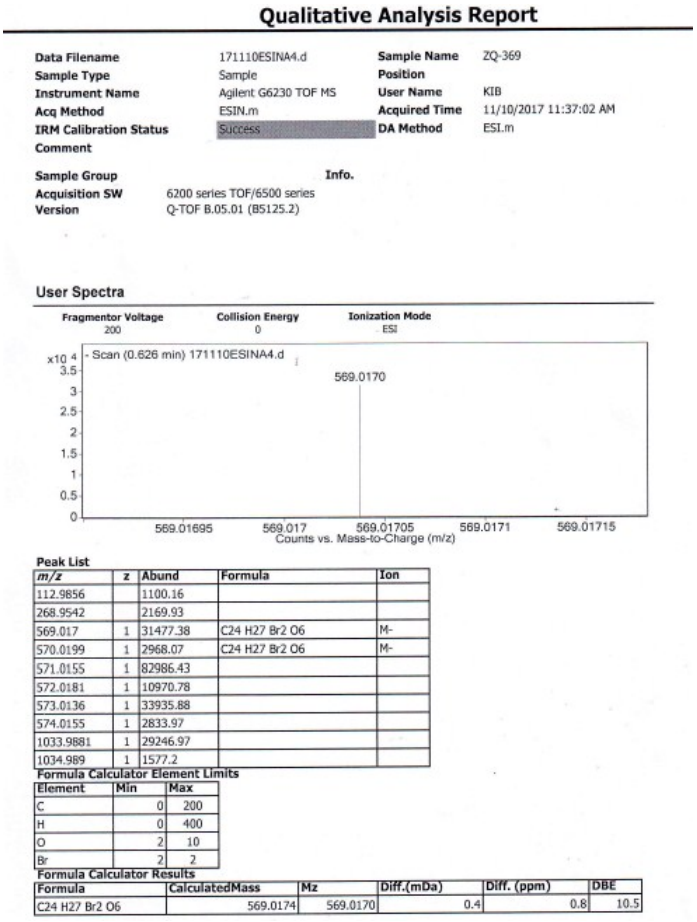


Figure 51S. Negative ESI-MS spectrum of compound **3e**



Qualitative Analysis Report

Data Filename	171110ESINA4.d	**Sample Name**	ZQ-369
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESIN.m	**Acquired Time**	11/10/2017 11:37:02 AM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI

Peak List

m/z	z	Abund	Formula	Ion
112.9856		1100.16		
268.9542		2169.93		
569.017	1	31477.38	C24 H27 Br2 O6	M-
570.0199	1	2968.07	C24 H27 Br2 O6	M-
571.0155	1	82986.43		
572.0181	1	10970.78		
573.0136	1	33935.88		
574.0155	1	2833.97		
1033.9881	1	29246.97		
1034.989	1	1577.2		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	2	10
Br	2	2

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C24 H27 Br2 O6	569.0174	569.0170	0.4	0.8	10.5

Figure 52S. Negative HR-ESIMS spectrum of compound **3e**